Foundations of Computational Materials Modelling
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Generation of crystals

Good afternoon. So, let us continue from where we left off in last class. We are almost nearing the end of the first module of this particular course where we will deal with space groups and then teach you how to interpret them and construct crystals through simple matlab... MATLAB programs.

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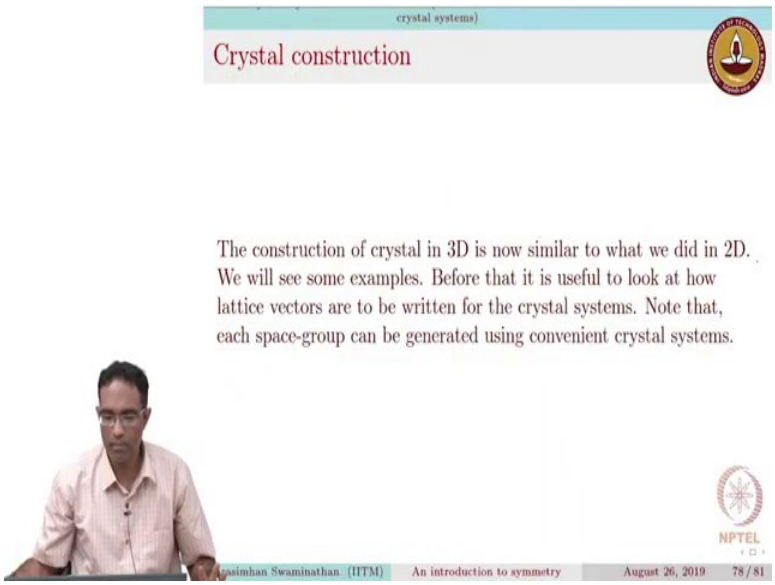

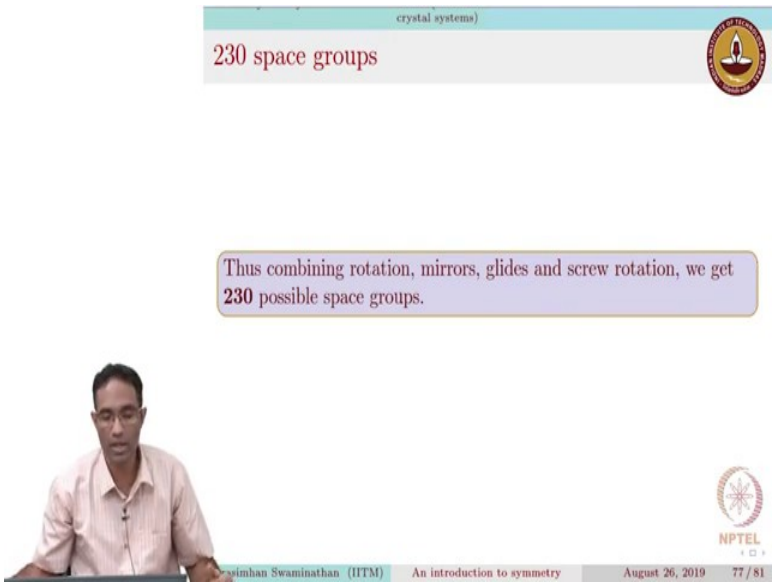

So, we stopped with realizing these 230 various space groups, depending upon the symmetry operators that are possible in 3 D space, including the screw rotation and the glide reflections.

And we highlighted, what those space groups were in yesterday's class. We just went through quickly what were the groups and what unit cell or crystal system can be used in order to construct them. So, now, we want to start constructing a couple of these crystals using a combination of what we already learned with regards to using the MATLAB program to construct some simple structures and also using the web page in order to identify appropriate Wyckoff positions.

So, that we know that these items are going to going to go. Depending upon the space that we will be dealing with, there might be some additional modifications that we will have to do to the code.

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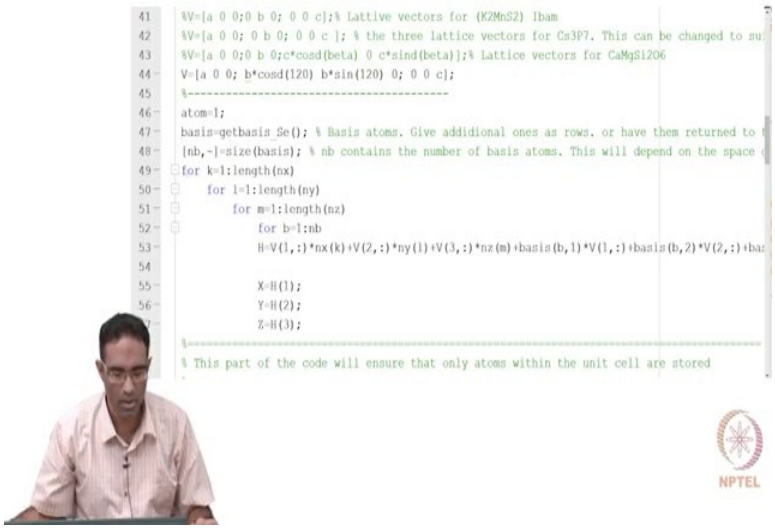

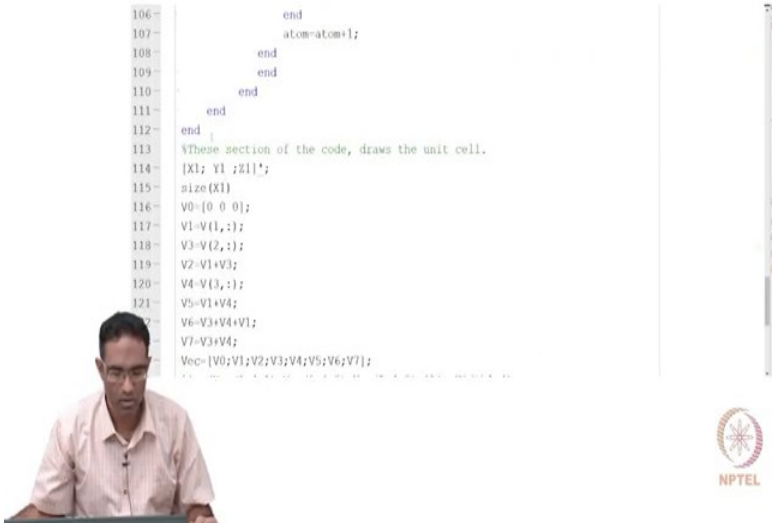

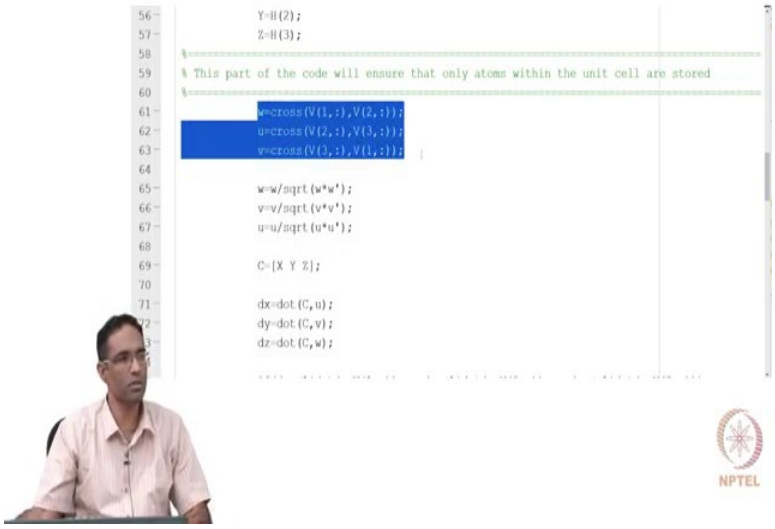

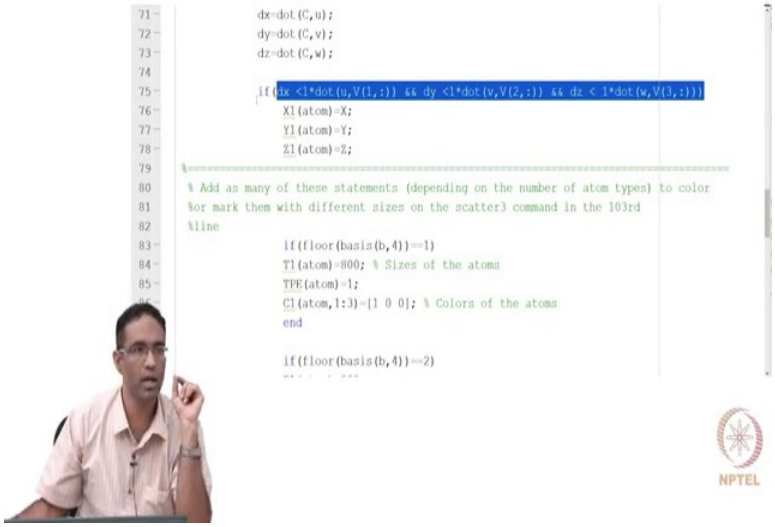

So, let us first open up the script that I just shared with you this morning, which is called us genlatt class exercise. And there are several different modifications to the original code that you had. The original code that you had was only able to create some FCC crystal structure. And another problem with that code was that you would be, you would not able to view the atoms that are belonging to just one unit cell. Usually it is convenient to view just one unit cell to see if you got it right.

So, there are some additional modifications that have been done to this code in order to make that possible. So, I will show you these lines where these modifications have been made. So, if you if you have seen this code a couple of times you will realize that most of these lines remain almost the same. So, beginning from line number 49 to 112, most of the stuff remains the same especially until line number 57. In the previous codes, I think you stopped with line

number 57 and ended all the 3 or 4 for loops and then simply printed out the atom numbers or the atom details.

But now what we want to do is we want to be checking whether this particular atom that has just been generated is actually lying within the unit cell. So, there are a couple of different lines that we have here. So, this is just based on simple analytical geometry. I do not want to be talking about the details as to why this works, but all I want you to do is, have lines 61 through 78 in your code.

You can have it 74, you can have it till 74 but after that you basically check, if you if you do till 74, you will be some generating certain values, and then you have the check, make a check here in line number 75. This is the line which is basically checking whether the particular point that you just generated lies within the unit cell or not.

Now, in this line number 75 you see these 1 is here, I am highlighting this 1 is here, you can actually increase these numbers to increase the number of points that will be printed out. So, if you just put 1, it will just put exactly those atoms that are going to lie inside the unit cell. If you put 1.1 for example, it might show you even those atoms which are belonging to the adjacent unit cells. So, depending upon that number there you can actually control you know, how you want to view the unit cell that you just generated.

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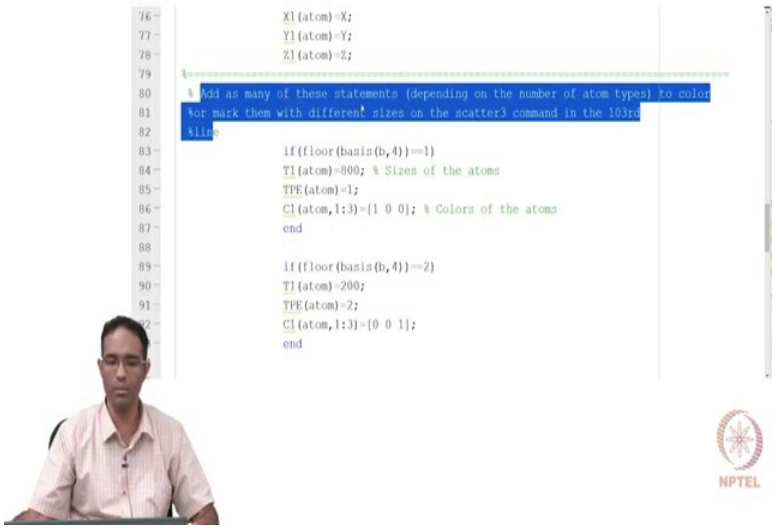

```
%or mark them with different sizes on the scatter3 command in the 103rd
%line
                if(floor(basis(b,4))==1)
                Tl(atom)=800; % Sizes of the atoms
                TPE(atom)=1;
                Cl(atom,1:3)=[1 0 0]; % Colors of the atoms
                end

                if(floor(basis(b,4))==2)
                Tl(atom)=200;
                TPE(atom)=2;
                Cl(atom,1:3)=[0 0 1];
                end


                if(floor(basis(b,4))==3)
                Tl(atom)=400;
                 TPE(atom)=3;
                Cl(atom,1:3)=[1 1 0];
```


```
                if(floor(basis(b,4))==3)
                Tl(atom)=400;
                 TPE(atom)=3;
                Cl(atom,1:3)=[1 1 0];
                end

                if(floor(basis(b,4))==4)
                  Tl(atom)=500;
                  TPE(atom)=4;
                  Cl(atom,1:3)=[1 0.5 2];
                end
                atom=atom+1;
            end
            end
        end
    end
end
%These section of the code, draws the unit cell.
[X1; Y1 ;Z1]';
```


```
%b=4.519;
%c=5.050;
%appropriate cell vectors
%V=[a 0 0;0 b 0; 0 0 c];%Lattice vectors for diamond (Fd-3m)
%V=[a 0 0;0 b 0; 0 0 c];% Lattice vectors for PdS (P4_2/m)
%V=[a 0 0;0 b 0; 0 0 c];% Lattive vectors for (K2MnS2) Ibam
%V=[a 0 0; 0 b 0; 0 0 c ]; % the three lattice vectors for Cs3P7. This can be changed to su
%V=[a 0 0;0 b 0;c*cosd(beta) 0 c*sind(beta)];% Lattice vectors for CaMgSi2O6
V=[a 0 0; b*cosd(120) b*sin(120) 0; 0 0 c];
%----------------------------------------
atom=1;
basis=getbasis_Se(); % Basis atoms. Give addidional ones as rows. or have them returned to t
[nb,~]=size(basis); % nb contains the number of basis atoms. This will depend on the space
for k=1:length(nx)
    for l=1:length(ny)
        for m=1:length(nz)
            for b=1:nb
            H=V(1,:)*nx(k)+V(2,:)*ny(l)+V(3,:)*nz(m)+basis(b,1)*V(1,:)+basis(b,2)*V(2,:)+bas
```

In addition to that, there are a couple of different lines here also which I have commented here, you know, add as many statements as required depending upon the number of atom types that you have. So, that you can color or mark them in different sizes and plot them nicely.

So, these are the various lines right here. Now, so there are some other modifications also which have been done to the basis array, which is returned by the get basis function. So, remember the get basis function, what does it do? It basically gives you the set of all the set of points that you wanted to print out n in fractional coordinates.

So, previously the basis array contained only what? Contain only 3 columns and as many rows as there were basis atoms is that right, did you all, do all remember that? It contained 3 x, it contain x factional x coordinate, fractional y coordinates and fractional z coordinates. And as many rows as there were basis atoms present in that particular crystal. Right now, what happens is that the basis atom contains one additional column which represents an integer 1, 2, 3, 4, so on and so forth, representing something some information on the atom, so that you can decide how to color it.

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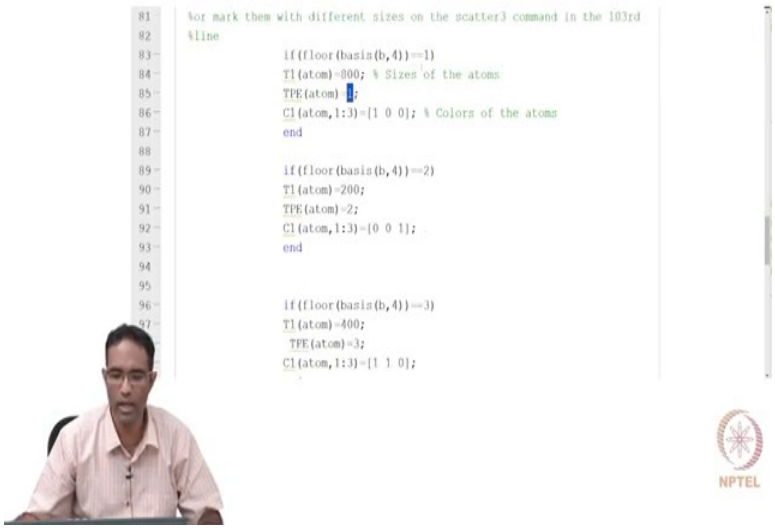

So, for example, basis fourth column, if you look at the eighty third line, I say floor of basis b, comma 4 is equal to 1. So, if it is atom type 1 and this would have been named in the get basis function. We would have name the bth basis fourth column as 1 for some atom. And if it is that atom that I want to give some size to it size to print out, so that I am able to control

the size of the circle that gets printed out in my MATLAB script. I am going to just say type of the atom as 1, so on and so forth.

You can keep playing with this and this one is basically the color 100 represents the RGB color for this particular atom and you can again play with this. So, if it is atom of type 2, then I can change the color, I can change the size if is atom of type 3, then I can have a different size, I can have a different color and you can add as many if statements as required, depending upon the number of atom types that you have and color them and plot them and have a good and visually inspect the crystal that you just generated.

So, this is something that should work for any crystal systems as long as you know how to construct it, and give the right basis for this and choose the right lattice vector.

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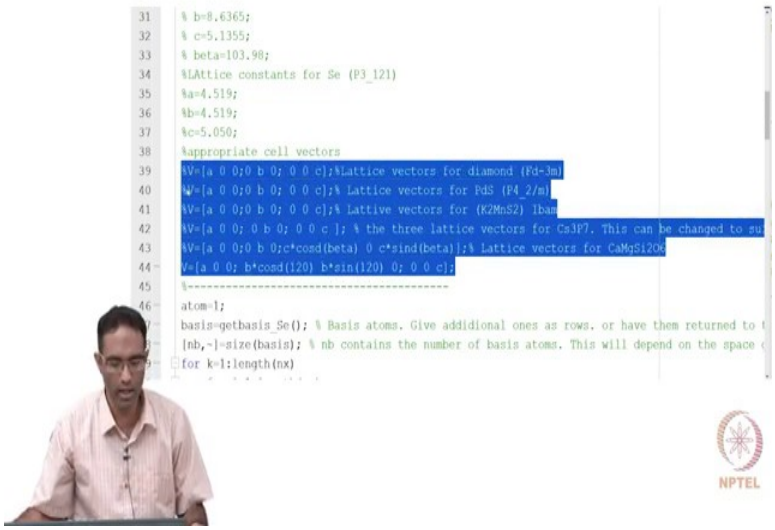

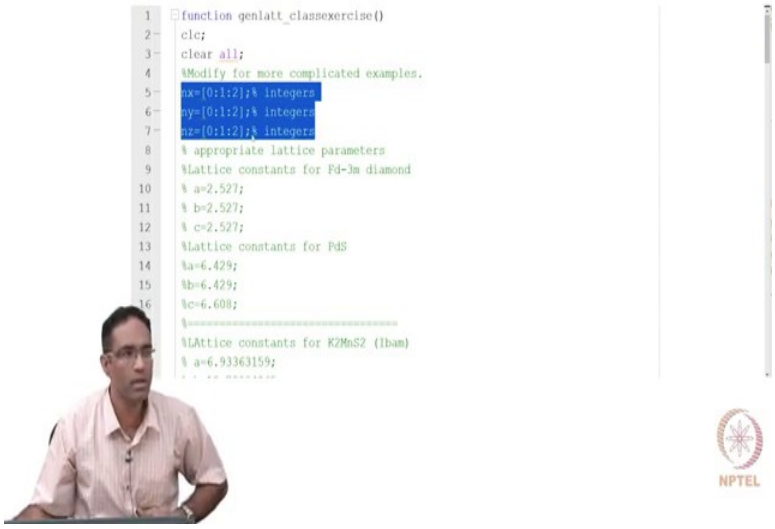

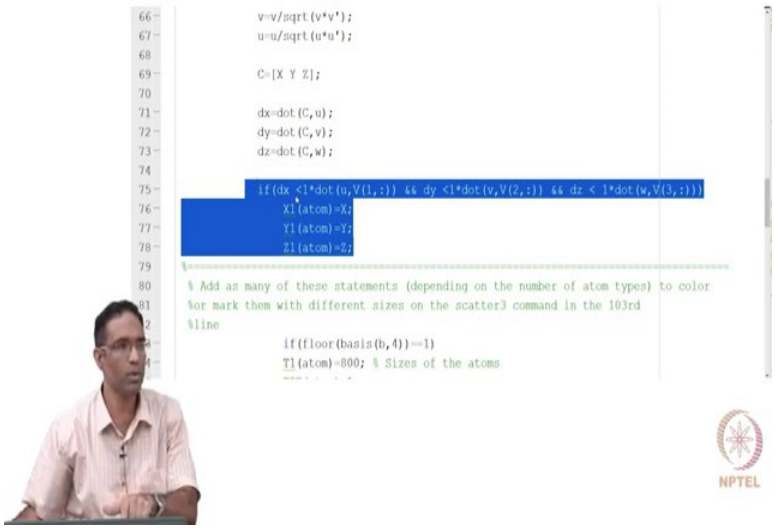

So, these are the various lattice vectors, which I am going to talk about today. You do not need so many as you can see, I have commented some and I am going to uncomment one by one, depending upon which crystal structure I am going to discuss, is that okay? So, the first thing that I want to discuss, so this is just a set of integers going from 0 to 2 or 0 to whatever and if you want to use this code in order to generate the data file, for example, for the LAMMPS program.

But in that case, it will not contain only one unit cell. It might contain large number of unit cells, you might want to analyze, you know 10 by 10 by 10 unit cells, then you might have to modify this number to 10, 10, 10 and then not have these statements, so it not have these statements, because this one will only store the atoms which will lie within the unit cell within one unit set or you can just put 10 here and then it will show all the atoms which is

lying within 10 unit cells. So, in this manner you can actually modify this program pretty quickly in order to get the right number of unit cells, control them and visualize them.

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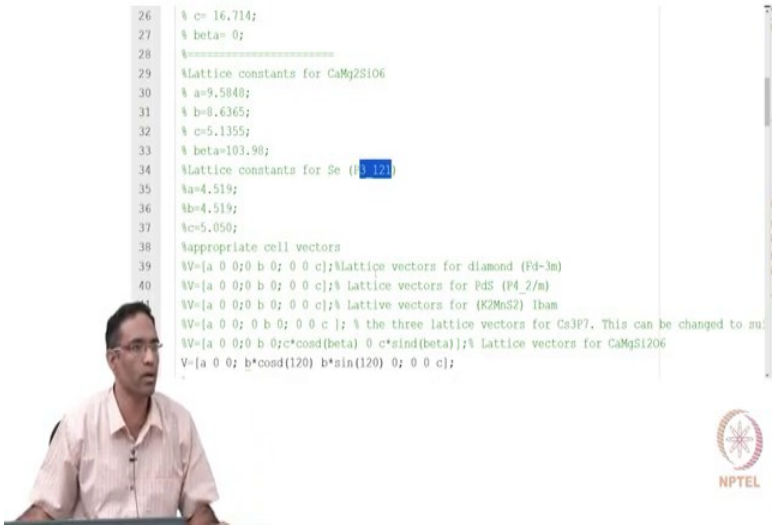

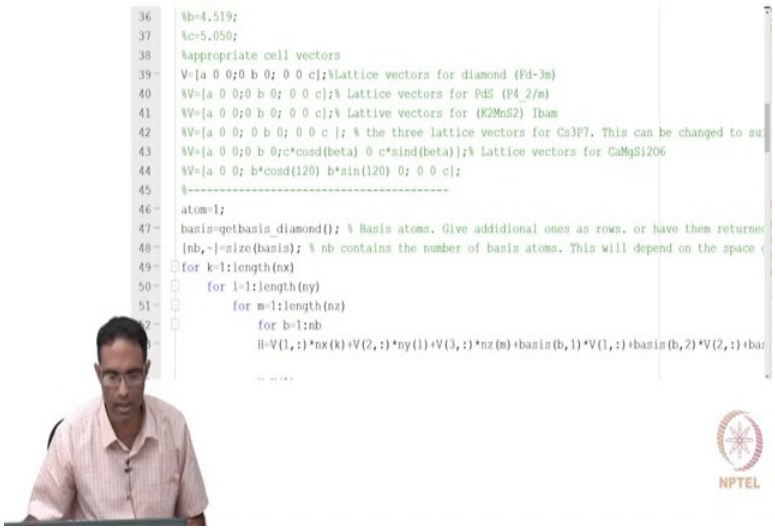

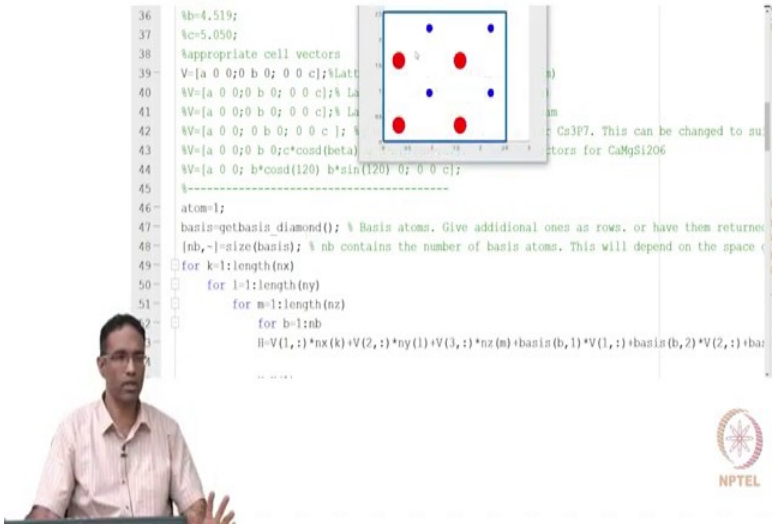

So, before we now, before doing anything more complicated, let us try to generate a simple structure and during this process we will learn a few things about the about centered lattices as well and how to use, how to generate Wyckoff positions for them as well. Yes?

Student: The code you uploaded does not have the Selenium part?

Professor: Yeah, and the one which I uploaded Selenium part is not there. I have later on added that to demonstrate construction of a crystal lattice with this space group P3 underscore 1 21. So, it is already but it is not there. I will teach you how to construct it. You can modify the code in order to do that, it is going to be quite simple.

The first one that I want to generate is now this I want to start with the diamond. So the diamond, so I just uncomment those lines. And I change this to diamond because this is what I have shared with you. I have not shared the get basis command with for the other crystal structures as well, I think I have shared with you only get basis underscore diamond. Is that right?

This morning, so now if you make these small changes basically uncomment the lattice constants for diamond, uncomment the lattice vectors for diamond and then get basis for diamond and click run, you should generate a structure and this is basically the diamond structure.ok? And you can, of course view this in different ways and this is the diamond structure.

How many of you are convinced that this looks like the diamond structure? If you have seen it before, you will know that this is the diamond structure. And I have colored these atoms

slightly differently. So, I have two different types of atoms here in a sense, they both are carbon, but I have just colored them intentionally differently to show you that they are of different types. So, what did I do in order to get this?

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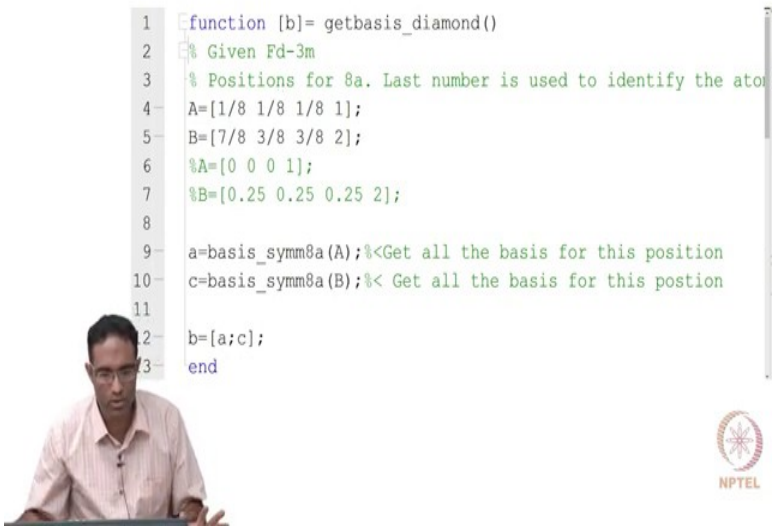

So, this is all the changes now, are going to be in the get basis diamond, file. So, we can open the get basis diamond file. So, this is a get basis diamond function and what do we need to give here? We need to give the basis, the various basis atoms, but the manner in which we have been doing this class. We first need to know the corresponding space group and the corresponding Wyckoff position to which the carbon atom is going to be located in the diamond structure. So, that will be given to us like I told you that is going to be given to us.

For the diamond carbon, the carbon is present at position 8a and it has the space group Fd 3 bar m. So, what does F mean?

Student: Face centered.

Professor: Face centered d mean?

Student: Diamond glide.

Professor: There is a diamond glide, so that is the reason why the d is used because that sort of a glide is present in diamond structures, 3 bar is 3 bar. And m is mirror. The third slot, that is the second slot after the F, basically contains a 3 Fd 3 bar, 3 bar which means that it is a what unit cell will you use?

Student: Cubic unit cell.

Professor: Cubic unit cell, so from that it should be clear that what, it should be clear what your lattice vectors are supposed to be, supposed to be a equal to b equal to c equal to some particular number and alpha equal to beta equal to gamma is equal to 90 degrees.

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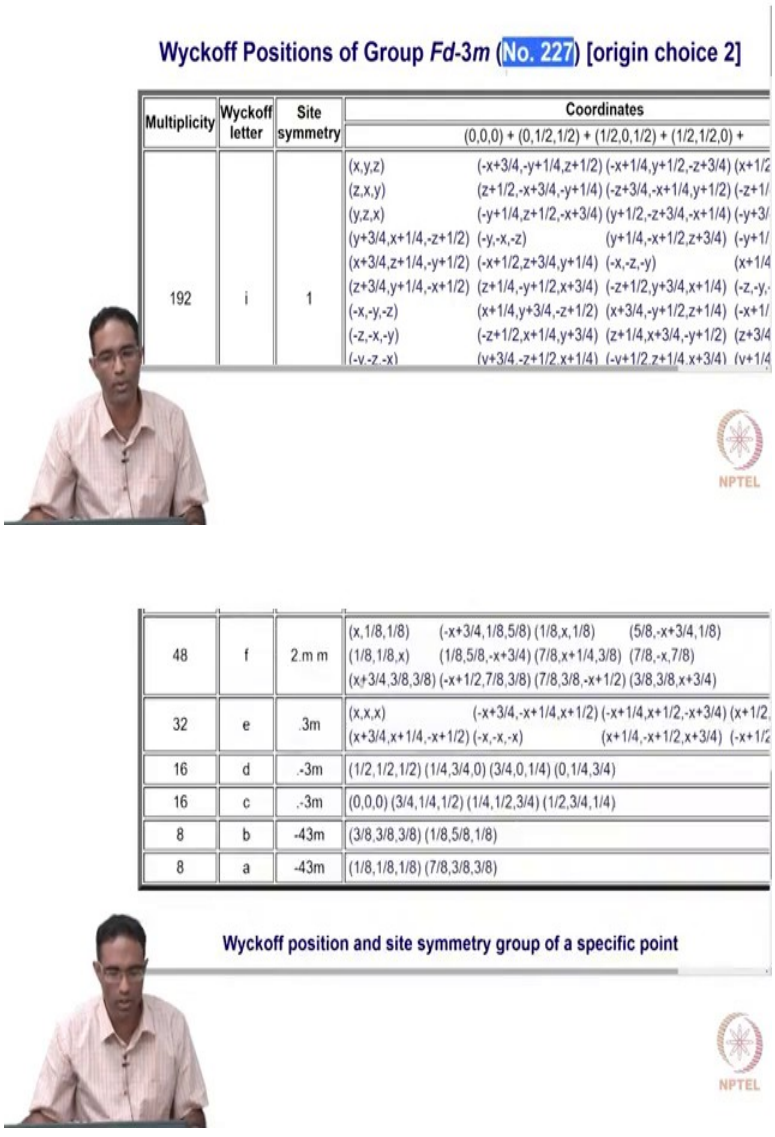

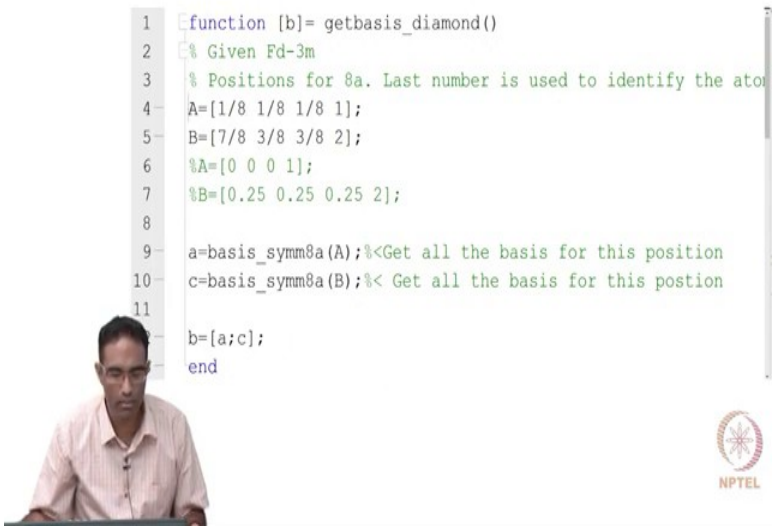

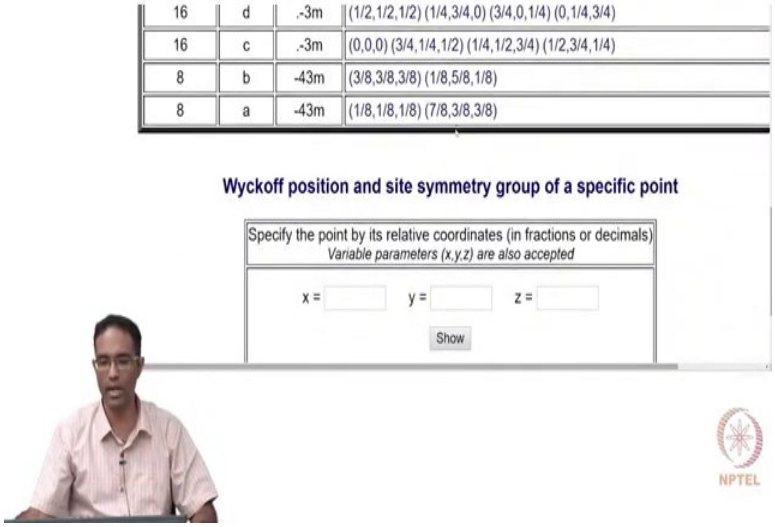

So, now let us go to our crystallographic website and look at how a space group Fd 3 bar m which is a number 227 and in that I said that it does belong into position 8a. So, at 8a and there is one atom at 1 by 8, 1, ok ? by 8, 1 by 8 and another one at 7 by 8, 3 by 8 and 3 by 8. So, what I do there is, I go to my MATLAB program and I give one atom at 1 by 8, 1 by 8, 1 by 8 followed by a 1, telling that that is of atom type 1 and then b is 7 by 8, 3 by 8, 3 by 8 and followed by a 2 indicating that, that is of atom type 2.

Now, it is not enough that I just do this because there are just 2 basis atoms but you will know that diamond structure has more than that inside one particular unit cell and you have just given 2 atoms right here. So, how do we generate the other atoms? And even in the even in the crystallographic website, you will not have anything else given right here, you just have these 2. But whenever you have the centered lattices that means those lattices which

begin with the f or I, right? or a or c, right?, like what would occur in a and c would occur in orthorhombic.

You would go to the top and you would see something like this 0, 0, 0 plus 0, half, half plus half, 0, half plus half, half, 0. So, if you took each of those points that were generated, that were given to you, to each of them, you have to add this, these centering coordinates to each, so to 0, 0, 0 that is to 1 by 8, 1 by 8, 1 by 8, I would have to add this.

So, I would generate 4 additional point and then to 7 b y 8, 3 by 8 and 3 by 8, I would have to add this then I would generate 4 additional points. Consequently, I have 8 different points present within the unit cell, which is why I have a multiplicity of 8 right here. So, note that is again done inside the get basis command. So, I say that 1 by 8, 1 by 8, 1 by 8, 1, b is 7 by 8, 3 by 8, 3 by 8, 2.

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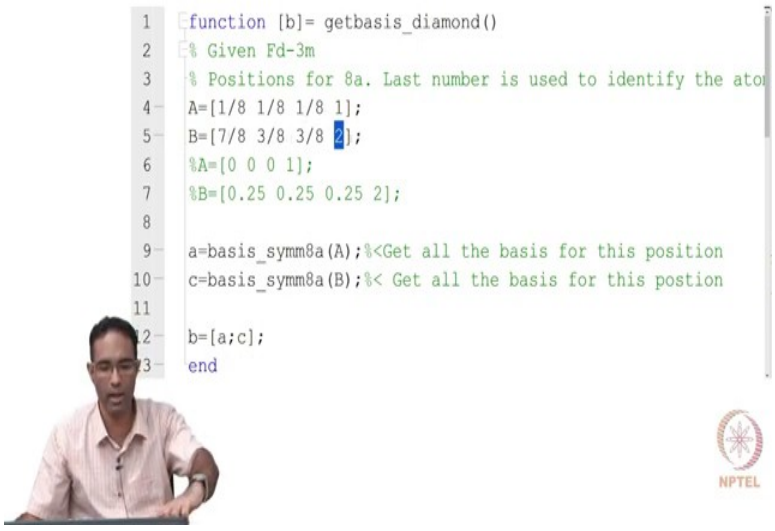

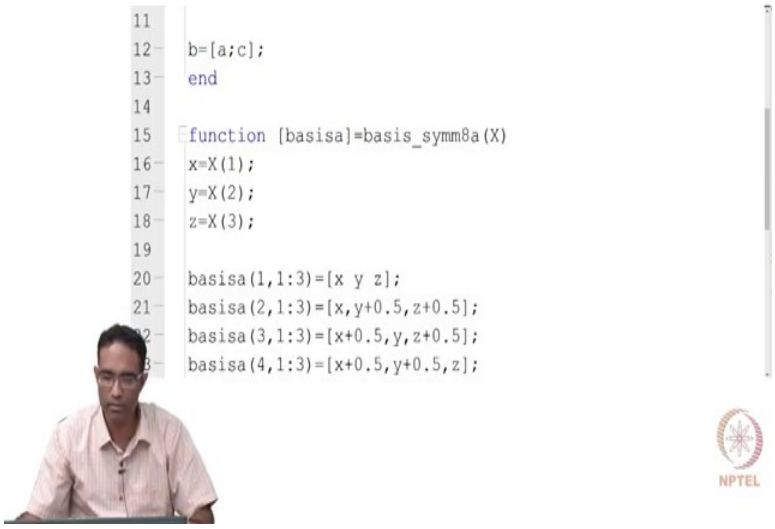

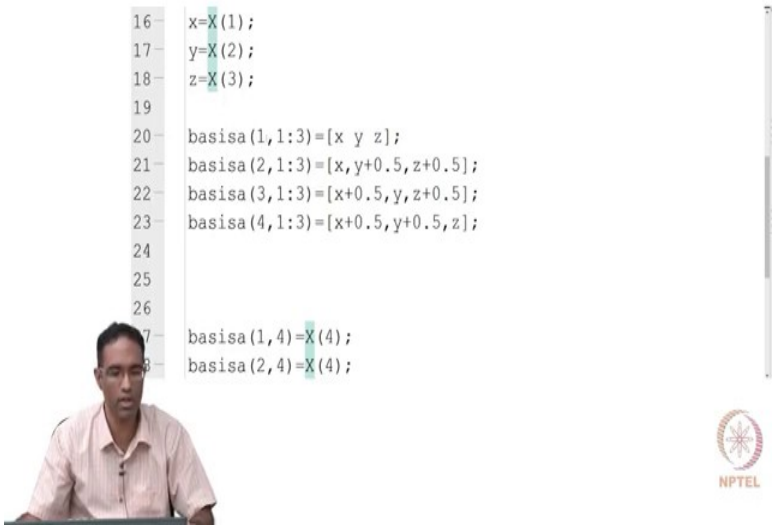

Then I have a new function called as basis underscore sym 8a. And what happens in that, what happens in that function? The following, so this is that function basis underscore sym 8a. It takes in the x, which is this entire thing, it is taken in the A array. So, it has taken that in the X right here and I say the X fraction coordinate is x of 1, y fraction coordinate is x of 2 and z fraction coordinate is x of 3 and I develop another array with by adding the appropriate components 0, 0, 0, half, 0 half, sorry 0 half, half, half, 0, half and half, half, 0 and generate 4, those 4 additional point for each of those things.

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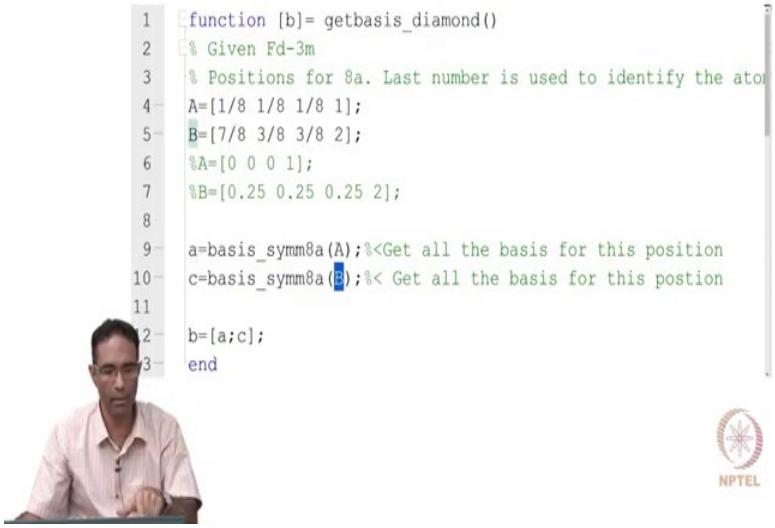

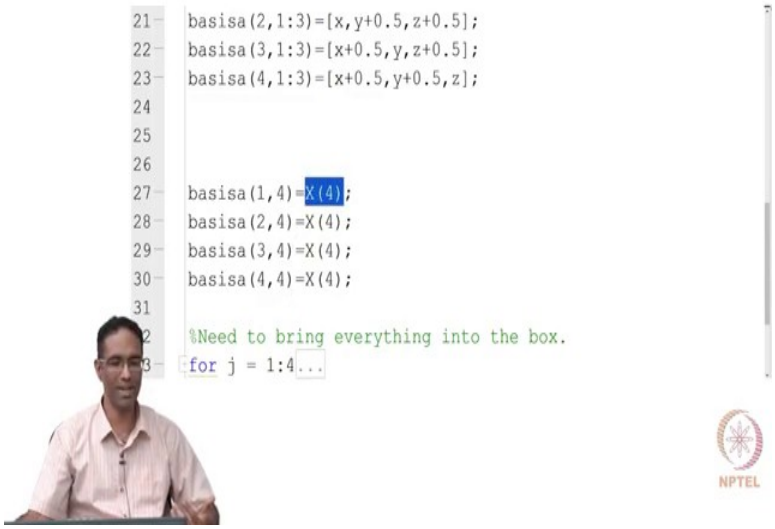

So, it is the first I give it to A, first I say basis under sym 8a A. So, this small a now will contain those 4 additional points, right?. Again, I do the same thing for the B where B is 7 by 8, 3 by 8, 3 by 8, 2 and I get that in this array C, so this a will contains 4 rows, c will contain 4 rows. The column vector will have to be retained, so all these atoms belong to this A type right 1. So, anything that goes into A, I will have to retain, x of 4 in the fourth column. So, basis a 1, 2, 3, 4, the fourth column will contain x of 4 and x of 4 is basically having 1.

Similarly, if you do for the Bth atom the x of 4 will now contain 2. Once I receive a and c, I am going to return a concatenated array of the basis atoms containing even the information as to what the atom type is to the main program. is that right ?

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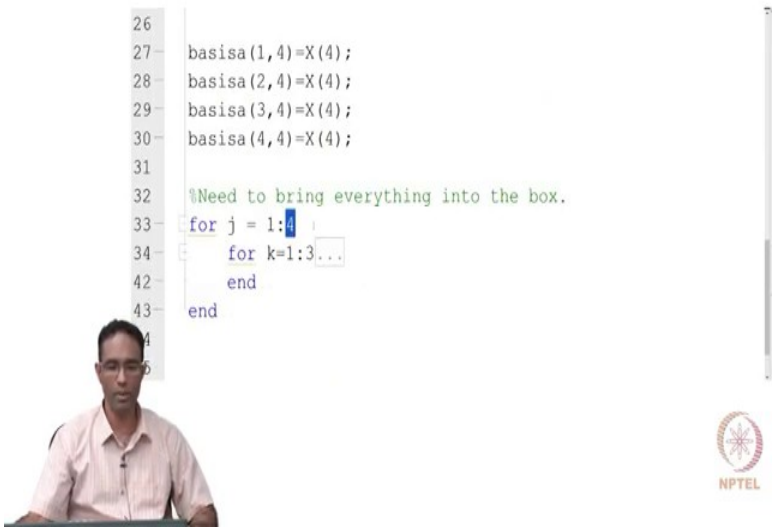
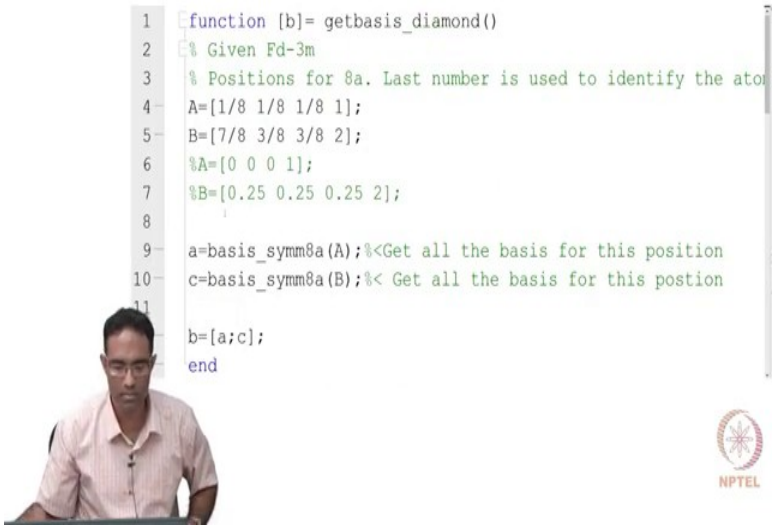
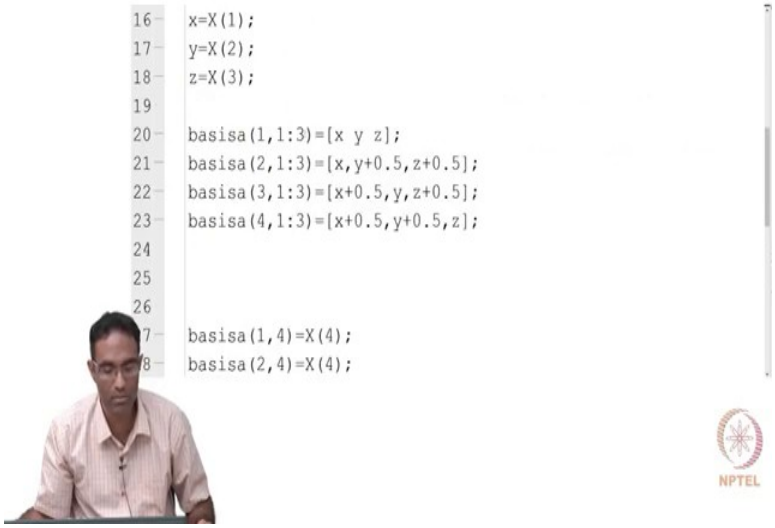






Now, in addition to this, there is something else just been done here. Sometimes, what can happen is, so 1 by 8, so 1 by 8 plus half, what is it going to be?

Student: 5 by 8

Professor: 1 by 8 plus half.

Student: 5 by 8.

Professor: 5 by 8, sometimes 7 by 8 plus half.

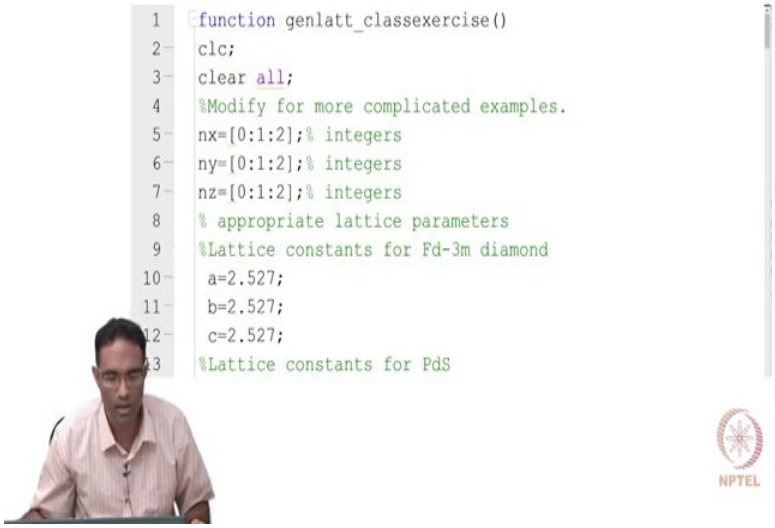
Student: 11 by 8.

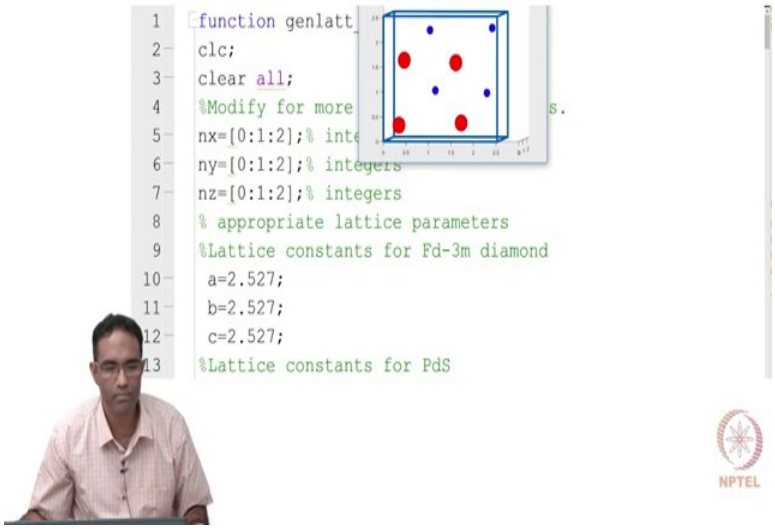
Professor: 11 by 8, it becomes greater than 1, correct? It becomes greater than 1. So, 7 by 8 plus half, somewhere you are going to do plus half becomes greater than 1. So, you have to keep track of these fractional coordinates which are actually going outside the unit cell and pull them back inside the unit cell. So, it becomes greater than on1e you will have to subtract 1. And at other instances, you may have negative x, negative y being specified.

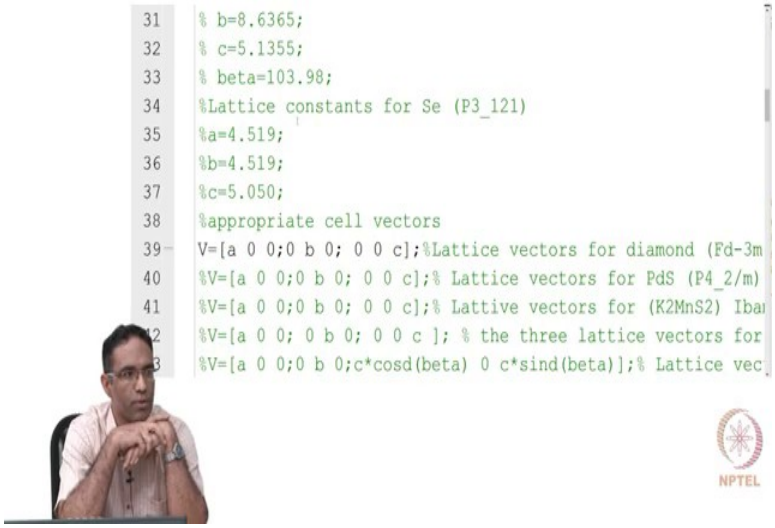
So, if it is having a negative value, you might have to add 1 to it to pull it back inside the unit cell. So, in the, after actually assigning all these rules for the basis a, we write a for loop which will basically see if it is less than 0, if the values of the kth column for all the 4 different atoms this 4 can, 4 depends on how many basis atoms are being generated for that particular position.

If it is less than 0, I will have to do 1 minus that. And if it is greater than 1, I will have to do that minus 1 to pull it back inside the unit cell. So, this is what is being done always, these things are pretty much boilerplate, you only have to change a few things here in order to generate your other crystals.

(Refer Slide Time: 18:08)

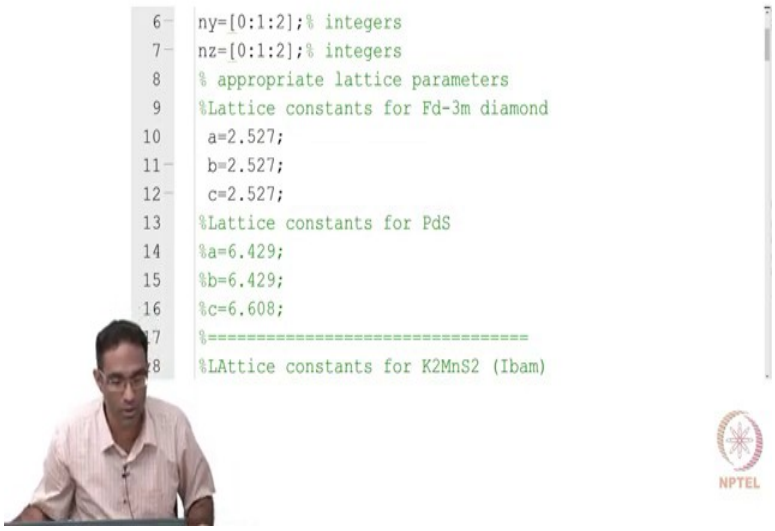


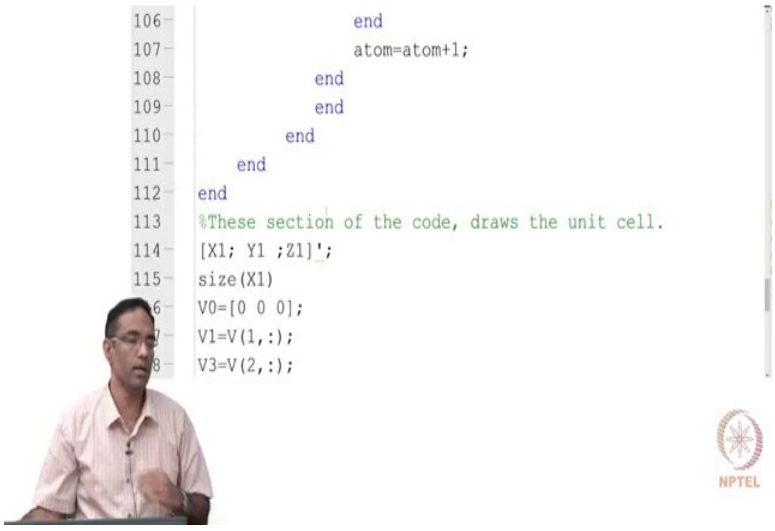




So, once you do this, you can go back and click run and you would generate your unit cell and the unit cell also is, all the unit cell vectors are also marked in the cells your unit cell is nicely marked here. And you can actually examine that and see if what you have generated is correct before you actually go ahead and generate the entire structure in order to perform some analysis using your molecular dynamics simulation software. So, this is the construction for simple diamond structure.

(Refer Slide Time: 18:44)

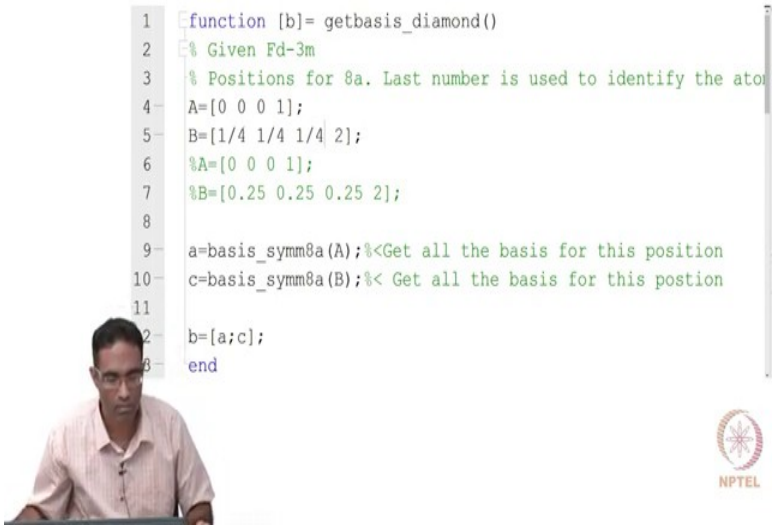


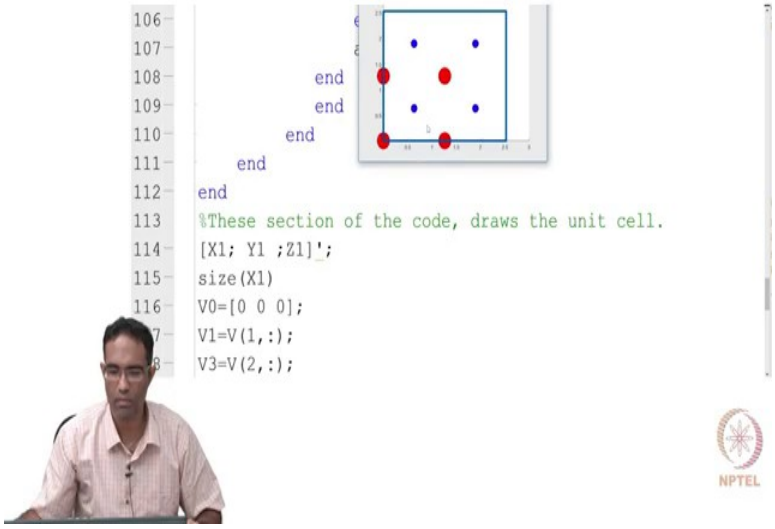


Now, we can go ahead and do so, now let us proceed to generate something a little bit more involved. I am going to try to do PdS before that let me show you something else with respect to diamond also. So, diamond sometimes when you see the Wyckoff position for the

diamond, they will just say that there is a there is an atom at 0, 0, 0 and there is another one at quarter, quarter, quarter. That is how the diamond structure looks.

(Refer Slide Time: 19:21)





How to select the group

The space groups are specified by their number as given in the *International Tables for Crystallography*, Vol. A. You can give this number, if you know it, or you can choose it from the table with the space group numbers and symbols if you click on the link **choose it**.

The available crystallographic data refer either to the standard/default setting of the chosen space group or to the so-called ITA Settings.

Please, enter the sequential number of group as given in *International Tables for Crystallography*, Vol. A or choose it: 227

Standard/Default Setting | Non Conventional Setting | ITA Settings

Bilbao Crystallographic Server → WYCKPOS → Wyckoff Positions Help

Wyckoff Positions of Group *Fd*-3*m* (No. 227) [origin choice 2]

Multiplicity	Wyckoff letter	Site symmetry	Coordinates			
			(0,0,0) + (0,1/2,1/2) + (1/2,0,1/2) + (1/2,1/2,0) +			
192	i	1	(x,y,z)	(-x+3/4,-y+1/4,z+1/2)	(-x+1/4,y+1/2,-z+3/4)	(x+1/2
			(z,x,y)	(z+1/2,-x+3/4,-y+1/4)	(-z+3/4,-x+1/4,y+1/2)	(-z+1/
			(y,z,x)	(-y+1/4,z+1/2,-x+3/4)	(y+1/2,-z+3/4,-x+1/4)	(-y+3/
			(y+3/4,x+1/4,-z+1/2)	(-y,-x,-z)	(y+1/4,-x+1/2,z+3/4)	(-y+1/
			(x+3/4,z+1/4,-y+1/2)	(-x+1/2,z+3/4,y+1/4)	(-x,-z,-y)	(x+1/4
			(z+3/4,y+1/4,-x+1/2)	(z+1/4,-y+1/2,x+3/4)	(-z+1/2,y+3/4,x+1/4)	(-z,-y,
			(-x,-y,-z)	(x+1/4,y+3/4,-z+1/2)	(x+3/4,-y+1/2,z+1/4)	(-x+1/
			(-z,-x,-y)	(-z+1/2,x+1/4,y+3/4)	(z+1/4,x+3/4,-y+1/2)	(z+3/4
			(-y,-z,-x)	(y+3/4,-z+1/2,x+1/4)	(-y+1/2,z+1/4,x+3/4)	(y+1/4

Please, enter the transformation:

Linear part			Origin shift
1	0	0	1/8
0	1	0	1/8
0	0	1	1/8

Change the basis

Bilbao Crystallographic Server
http://www.cryst.ehu.es

For comments, please mail to
administrador.bcs@ehu.eus

Multiplicity	Wyckoff letter	Site symmetry (std.)	Coordinates	
			Standard/Default setting	
			(0,0,0) + (0,1/2,1/2) + (1/2,0,1/2) + (1/2,1/2,0) +	(0,0,0) +
192	i	1	(x,y,z) (-x+3/4,-y+1/4,z+1/2) (-x+1/4,y+1/2,-z+3/4) (x+1/2,-y+3/4,-z+1/4)	(x+7/8,y+7/8,z+7/8) (-x+5/8
			(z,x,y) (z+1/2,-x+3/4,-y+1/4) (-z+3/4,-x+1/4,y+1/2) (-z+1/4,x+1/2,-y+3/4)	(z+7/8,x+7/8,y+7/8) (z+3/8,
			(y,z,x) (-y+1/4,z+1/2,-x+3/4) (y+1/2,-z+3/4,-x+1/4) (-y+3/4,-z+1/4,x+1/2)	(y+7/8,z+7/8,x+7/8) (-y+1/8
			(y+3/4,x+1/4,-z+1/2) (-y,-x,-z) (y+1/4,-x+1/2,z+3/4) (-y+1/2,x+3/4,z+1/4)	(y+5/8,x+1/8,-z+3/8) (-y+7/8
			(x+3/4,z+1/4,-y+1/2) (-x+1/2,z+3/4,y+1/4) (-x,-z,-y) (x+1/4,-z+1/2,y+3/4)	(x+5/8,z+1/8,-y+3/8) (-x+3/8
			(z+3/4,y+1/4,-x+1/2) (z+1/4,-y+1/2,x+3/4) (-z+1/2,y+3/4,x+1/4) (-z,-y,-x)	(z+5/8,y+1/8,-x+3/8) (z+1/8,
			(-x,-y,-z) (x+1/4,y+3/4,-z+1/2) (x+3/4,-y+1/2,z+1/4) (-x+1/2,y+1/4,z+3/4)	(-x+7/8,-y+7/8,-z+7/8) (x+1/8,
			(-z,-x,-y) (-z+1/2,x+1/4,y+3/4) (z+1/4,x+3/4,-y+1/2) (z+3/4,-x+1/2,y+1/4)	(-z+7/8,-x+7/8,-y+7/8) (-z+3/8
			(-y,-z,-x) (y+3/4,-z+1/2,x+1/4) (-y+1/2,z+1/4,x+3/4) (y+1/4,z+3/4,-x+1/2)	(-y+7/8,-z+7/8,-x+7/8) (y+5/8,
			(-y+1/4,-x+3/4,z+1/2) (y,x,z) (-y+3/4,x+1/2,-z+1/4) (y+1/2,-x+1/4,-z+3/4)	(-y+1/8,-x+5/8,z+3/8) (y+7/8,
			(-x+1/4,-z+3/4,y+1/2) (x+1/2,-z+1/4,-y+3/4) (x,z,y) (-x+3/4,z+1/2,-y+1/4)	(-x+1/8,-z+5/8,y+3/8) (x+3/8,
			(-z+1/4,-y+3/4,x+1/2) (-z+3/4,y+1/2,-x+1/4) (z+1/2,-y+1/4,-x+3/4) (z,y,x)	(-z+1/8,-y+5/8,x+3/8) (-z+5/8
96	h	.2	(0,y,-y) (3/4,-y+1/4,-y+1/2) (1/4,y+1/2,y+3/4) (1/2,-y+3/4,y+1/4)	(7/8,y+7/8,-y+7/8) (5/8,-y+1/8
			(-y,0,y) (-y+1/2,3/4,-y+1/4) (y+3/4,1/4,y+1/2) (y+1/4,1/2,-y+3/4)	(-y+7/8,7/8,y+7/8) (-y+3/8,5/8
			(y,-y,0) (-y+1/4,-y+1/2,3/4) (y+1/2,y+3/4,1/4) (-y+3/4,y+1/4,1/2)	(y+7/8,-y+7/8,7/8) (-y+1/8,-y+
			(0,-y,y) (1/4,y+3/4,y+1/2) (3/4,-y+1/2,-y+1/4) (1/2,y+1/4,-y+3/4)	(7/8,-y+7/8,y+7/8) (1/8,y+5/8,
			(y,0,-y) (y+1/2,1/4,y+3/4) (-y+1/4,3/4,-y+1/2) (-y+3/4,1/2,y+1/4)	(y+7/8,7/8,-y+7/8) (y+3/8,1/8,
			(-y,y,0) (y+3/4,y+1/2,1/4) (-y+1/2,-y+1/4,3/4) (y+1/4,-y+3/4,1/2)	(-y+7/8,y+7/8,7/8) (y+5/8,y+3/
			(x,x,z) (-x+3/4,-x+1/4,z+1/2) (-x+1/4,x+1/2,-z+3/4) (x+1/2,-x+3/4,-z+1/4)	(x+7/8,x+7/8,z+7/8) (-x+5/8,-

1/2,-z+1/4,-y+3/4) (x,z,y) (-x+3/4,z+1/2,-y+1/4)	(-x+1/8,-z+5/8,y+3/8) (x+3/8,-z+1/8,-y+5/8) (x+7/8,z+7/8,y+7/8) (-x+5/8,z+3/8,-y+1/8)
+3/4,y+1/2,-x+1/4) (z+1/2,-y+1/4,-x+3/4) (z,y,x)	(-z+1/8,-y+5/8,x+3/8) (-z+5/8,y+3/8,-x+1/8) (z+3/8,-y+1/8,-x+5/8) (z+7/8,y+7/8,x+7/8)
?) (1/4,y+1/2,y+3/4) (1/2,-y+3/4,y+1/4)	(7/8,y+7/8,-y+7/8) (5/8,-y+1/8,-y+3/8) (1/8,y+3/8,y+5/8) (3/8,-y+5/8,y+1/8)
l) (y+3/4,1/4,y+1/2) (y+1/4,1/2,-y+3/4)	(-y+7/8,7/8,y+7/8) (-y+3/8,5/8,-y+1/8) (y+5/8,1/8,y+3/8) (y+1/8,3/8,-y+5/8)
l) (y+1/2,y+3/4,1/4) (-y+3/4,y+1/4,1/2)	(y+7/8,-y+7/8,7/8) (-y+1/8,-y+3/8,5/8) (y+3/8,y+5/8,1/8) (-y+5/8,y+1/8,3/8)
(3/4,-y+1/2,-y+1/4) (1/2,y+1/4,-y+3/4)	(7/8,-y+7/8,y+7/8) (1/8,y+5/8,y+3/8) (5/8,-y+3/8,-y+1/8) (3/8,y+1/8,-y+5/8)
(-y+1/4,3/4,-y+1/2) (-y+3/4,1/2,y+1/4)	(y+7/8,7/8,-y+7/8) (y+3/8,1/8,y+5/8) (-y+1/8,5/8,-y+3/8) (-y+5/8,3/8,y+1/8)
(-y+1/2,-y+1/4,3/4) (y+1/4,-y+3/4,1/2)	(-y+7/8,y+7/8,7/8) (y+5/8,y+3/8,1/8) (-y+3/8,-y+1/8,5/8) (y+1/8,-y+5/8,3/8)
3/4,-x+1/4,z+1/2) (-x+1/4,x+1/2,-z+3/4) (x+1/2,-x+3/4,-z+1/4)	(x+7/8,x+7/8,z+7/8) (-x+5/8,-x+1/8,z+3/8) (-x+1/8,x+3/8,-z+5/8) (x+3/8,-x+5/8,-z+1/8)
1/2,-x+3/4,-x+1/4) (-z+3/4,-x+1/4,x+1/2) (-z+1/4,x+1/2,-x+3/4)	(z+7/8,x+7/8,x+7/8) (z+3/8,-x+5/8,-x+1/8) (-z+5/8,-x+1/8,x+3/8) (-z+1/8,x+3/8,-x+5/8)
1/4,z+1/2,-x+3/4) (x+1/2,-z+3/4,-x+1/4) (-x+3/4,-z+1/4,x+1/2)	(x+7/8,z+7/8,x+7/8) (-x+1/8,z+3/8,-x+5/8) (x+3/8,-z+5/8,-x+1/8) (-x+5/8,-z+1/8,x+3/8)
x,-z) (x+1/4,-x+1/2,z+3/4) (-x+1/2,x+3/4,z+1/4)	(x+5/8,x+1/8,-z+3/8) (-x+7/8,-x+7/8,-z+7/8) (x+1/8,-x+3/8,z+5/8) (-x+3/8,x+5/8,z+1/8)
1/2,z+3/4,x+1/4) (-x,-z,-x) (x+1/4,-z+1/2,x+3/4)	(x+5/8,z+1/8,-x+3/8) (-x+3/8,z+5/8,x+1/8) (-x+7/8,-z+7/8,-x+7/8) (x+1/8,-z+3/8,x+5/8)
l/4,-x+1/2,x+3/4) (-z+1/2,x+3/4,x+1/4) (-z,-x,-x)	(z+5/8,x+1/8,-x+3/8) (z+1/8,-x+3/8,x+5/8) (-z+3/8,x+5/8,x+1/8) (-z+7/8,-x+7/8,-x+7/8)
8,5/8) (1/8,x,1/8) (5/8,-x+3/4,1/8)	(x+7/8,0,0) (-x+5/8,0,1/2) (0,x+7/8,0) (1/2,-x+5/8,0)
+3/4) (7/8,x+1/4,3/8) (7/8,-x,7/8)	(0,0,x+7/8) (0,1/2,-x+5/8) (3/4,x+1/8,1/4) (3/4,-x+7/8,3/4)
8,3/8) (7/8,3/8,-x+1/2) (3/8,3/8,x+3/4)	(x+5/8,1/4,1/4) (-x+3/8,3/4,1/4) (3/4,1/4,-x+3/8) (1/4,1/4,x+5/8)
3/4,-x+1/4,x+1/2) (-x+1/4,x+1/2,-x+3/4) (x+1/2,-x+3/4,-x+1/4)	(x+7/8,x+7/8,x+7/8) (-x+5/8,-x+1/8,x+3/8) (-x+1/8,x+3/8,-x+5/8) (x+3/8,-x+5/8,-x+1/8)
x,-x) (x+1/4,-x+1/2,x+3/4) (-x+1/2,x+3/4,x+1/4)	(x+5/8,x+1/8,-x+3/8) (-x+7/8,-x+7/8,-x+7/8) (x+1/8,-x+3/8,x+5/8) (-x+3/8,x+5/8,x+1/8)
3/4,0,1/4) (0,1/4,3/4)	(3/8,3/8,3/8) (1/8,5/8,7/8) (5/8,7/8,1/8) (7/8,1/8,5/8)
1/2,3/4) (1/2,3/4,1/4)	(7/8,7/8,7/8) (5/8,1/8,3/8) (1/8,3/8,5/8) (3/8,5/8,1/8)

(-y+1/2,-y+1/4,3/4) (y+1/4,-y+3/4,1/2)	(-y+7/8,y+7/8,7/8) (y+5/8,y+3/8,1/8) (-y+3/8,-y+1/8,5/8) (y+1/8,-y+5/8,3/8)
3/4,-x+1/4,z+1/2) (-x+1/4,x+1/2,-z+3/4) (x+1/2,-x+3/4,-z+1/4)	(x+7/8,x+7/8,z+7/8) (-x+5/8,-x+1/8,z+3/8) (-x+1/8,x+3/8,-z+5/8) (x+3/8,-x+5/8,-z+1/8)
1/2,-x+3/4,-x+1/4) (-z+3/4,-x+1/4,x+1/2) (-z+1/4,x+1/2,-x+3/4)	(z+7/8,x+7/8,x+7/8) (z+3/8,-x+5/8,-x+1/8) (-z+5/8,-x+1/8,x+3/8) (-z+1/8,x+3/8,-x+5/8)
1/4,z+1/2,-x+3/4) (x+1/2,-z+3/4,-x+1/4) (-x+3/4,-z+1/4,x+1/2)	(x+7/8,z+7/8,x+7/8) (-x+1/8,z+3/8,-x+5/8) (x+3/8,-z+5/8,-x+1/8) (-x+5/8,-z+1/8,x+3/8)
x,-z) (x+1/4,-x+1/2,z+3/4) (-x+1/2,x+3/4,z+1/4)	(x+5/8,x+1/8,-z+3/8) (-x+7/8,-x+7/8,-z+7/8) (x+1/8,-x+3/8,z+5/8) (-x+3/8,x+5/8,z+1/8)
1/2,z+3/4,x+1/4) (-x,-z,-x) (x+1/4,-z+1/2,x+3/4)	(x+5/8,z+1/8,-x+3/8) (-x+3/8,z+5/8,x+1/8) (-x+7/8,-z+7/8,-x+7/8) (x+1/8,-z+3/8,x+5/8)
l/4,-x+1/2,x+3/4) (-z+1/2,x+3/4,x+1/4) (-z,-x,-x)	(z+5/8,x+1/8,-x+3/8) (z+1/8,-x+3/8,x+5/8) (-z+3/8,x+5/8,x+1/8) (-z+7/8,-x+7/8,-x+7/8)
8,5/8) (1/8,x,1/8) (5/8,-x+3/4,1/8)	(x+7/8,0,0) (-x+5/8,0,1/2) (0,x+7/8,0) (1/2,-x+5/8,0)
+3/4) (7/8,x+1/4,3/8) (7/8,-x,7/8)	(0,0,x+7/8) (0,1/2,-x+5/8) (3/4,x+1/8,1/4) (3/4,-x+7/8,3/4)
8,3/8) (7/8,3/8,-x+1/2) (3/8,3/8,x+3/4)	(x+5/8,1/4,1/4) (-x+3/8,3/4,1/4) (3/4,1/4,-x+3/8) (1/4,1/4,x+5/8)
3/4,-x+1/4,x+1/2) (-x+1/4,x+1/2,-x+3/4) (x+1/2,-x+3/4,-x+1/4)	(x+7/8,x+7/8,x+7/8) (-x+5/8,-x+1/8,x+3/8) (-x+1/8,x+3/8,-x+5/8) (x+3/8,-x+5/8,-x+1/8)
x,-x) (x+1/4,-x+1/2,x+3/4) (-x+1/2,x+3/4,x+1/4)	(x+5/8,x+1/8,-x+3/8) (-x+7/8,-x+7/8,-x+7/8) (x+1/8,-x+3/8,x+5/8) (-x+3/8,x+5/8,x+1/8)
3/4,0,1/4) (0,1/4,3/4)	(3/8,3/8,3/8) (1/8,5/8,7/8) (5/8,7/8,1/8) (7/8,1/8,5/8)
1/2,3/4) (1/2,3/4,1/4)	(7/8,7/8,7/8) (5/8,1/8,3/8) (1/8,3/8,5/8) (3/8,5/8,1/8)
	(1/4,1/4,1/4) (0,1/2,0)
	(0,0,0) (3/4,1/4,1/4)

[Transformation matrix]

So, does this change anything here? Sorry 0, 0, 0, it is still a diamond structure. This is still a diamond structure, all that the crystallographic web page showed us was the fractional coordinate with respect to some other origin. We can always shift to the origin in order to get the appropriate the Wyckoff positions the X, Y, Z, fraction coordinate for a given Wyckoff position.

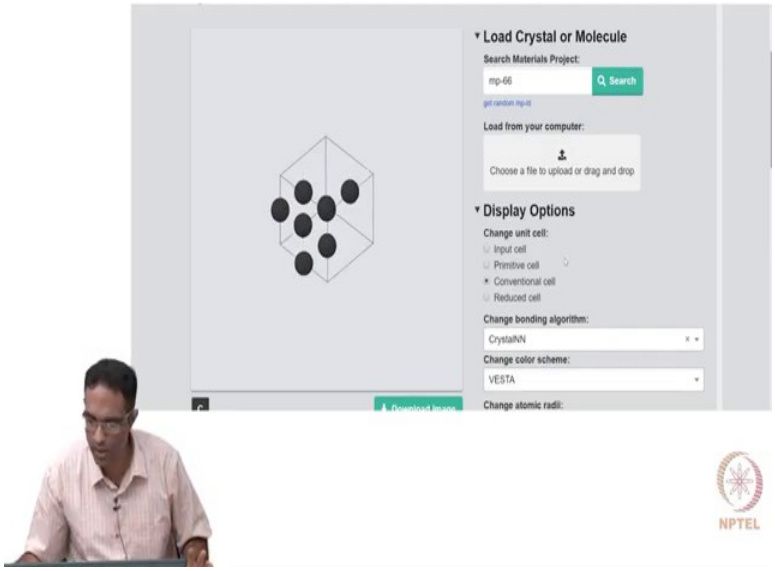
The website, the same website can also give us the new sets of Wyckoff position for shifted coordinate. So, for example, right now, I clicked the standard or default setting. When I click the standard or default setting I got one set of Wyckoff positions like X, Y, Z coordinates for different positions.

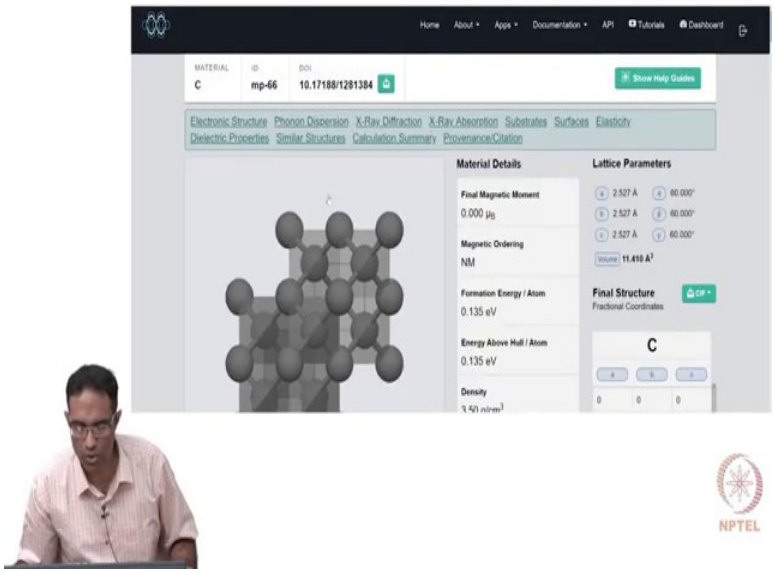
I may be able to do it for some other arbitrary non-conventional origin by simply specifying a origin shift. So, where I went there was I went a non-conventional setting. And I said, I want to shift the origin to 1 by 8, 1 by 8, 1 by 8 and then say change the basis.

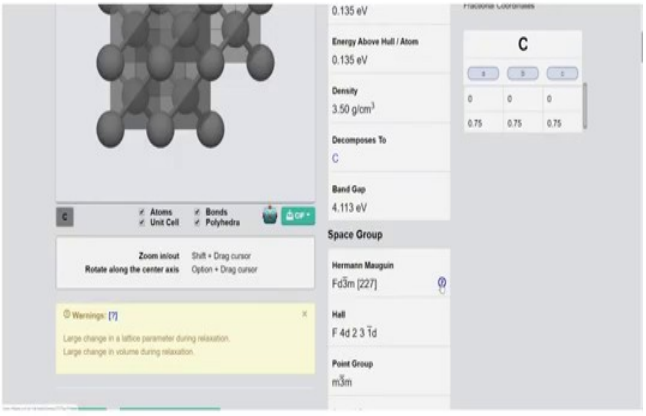
If I did that, you see that now, I will have one table on the left hand side showing the standard or default setting, and one table on the right, showing the corresponding X, Y, Z coordinates with the shifted origin. And in this case, I will have an atom 0, 0, 0 and another one at 3 quarters, 1 quarter and 1 quarter, which is what people are generally used to whenever they are dealing with diamond.

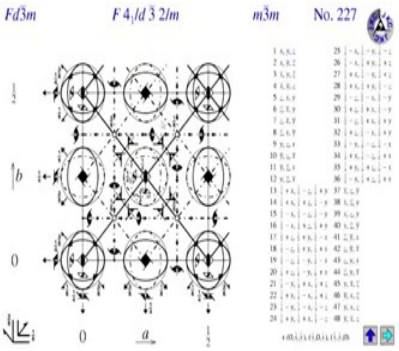
So, in this manner, whenever you are constructing the, these crystal structures with the crystallographic website, you need to be aware as to where the origin has been placed. And you need to at least not get confused whether the structure you are generating and the structure that you think you should get, whether they are same or whether they are different, it is something that you should keep checking.

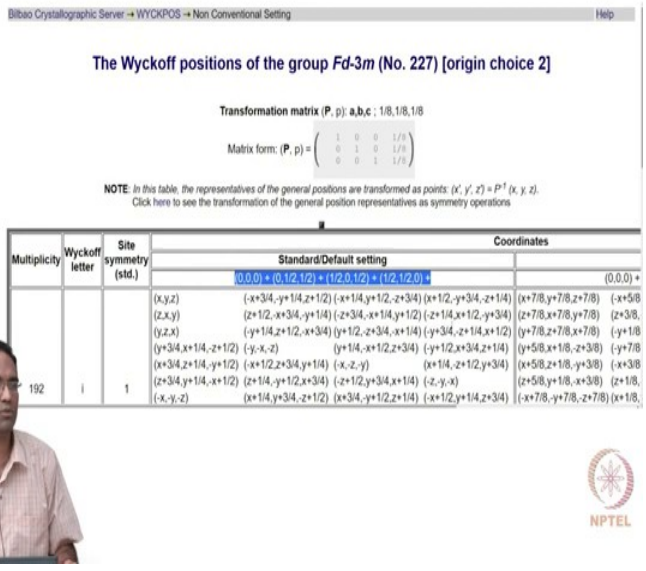
(Refer Slide Time: 22:04)






0.135 eV
Energy Above Hull / Atom
0.135 eV
Density
3.50 g/cm3
Decomposes To
C
Band Gap
4.113 eV
Space Group
Hermann Mauguin
Fd3̄m [227]
Hall
F 4d 2 3 1̄d
Point Group
m3̄m
C
Atoms
Unit Cell
Bonds
Polyhedra
Zoom in/out
Shift + Drag cursor
Rotate along the center axis
Option + Drag cursor
Warnings: [7]
Large change in a lattice parameter during relaxation.
Large change in volume during relaxation.


Fd3̄m
F 4₁/d 3̄ 2/m
m3̄m
No. 227


Bilbao Crystallographic Server → WYCKPOS → Non Conventional Setting
Help
The Wyckoff positions of the group Fd-3m (No. 227) [origin choice 2]
Transformation matrix (P, p): a,b,c ; 1/8,1/8,1/8
Matrix form: (P, p) =
NOTE: In this table, the representatives of the general positions are transformed as points: (x', y', z') = P⁻¹ (x, y, z).
Click here to see the transformation of the general position representatives as symmetry operations
Multiplicity
Wyckoff letter
Site symmetry (std.)
Coordinates
Standard/Default setting
(0,0,0) + (0,1/2,1/2) + (1/2,0,1/2) + (1/2,1/2,0) +
(0,0,0) +
192
i
1
(x,y,z) (-x+3/4,-y+1/4,z+1/2) (-x+1/4,y+1/2,-z+3/4) (x+1/2,-y+3/4,-z+1/4) (x+7/8,y+7/8,z+7/8) (-x+5/8
(z,x,y) (z+1/2,-x+3/4,-y+1/4) (-z+3/4,-x+1/4,y+1/2) (-z+1/4,x+1/2,-y+3/4) (z+7/8,x+7/8,y+7/8) (z+3/8,
(y,z,x) (-y+1/4,z+1/2,-x+3/4) (y+1/2,-z+3/4,-x+1/4) (-y+3/4,-z+1/4,x+1/2) (y+7/8,z+7/8,x+7/8) (-y+1/8
(y+3/4,x+1/4,-z+1/2) (-y,-x,-z) (y+1/4,-x+1/2,z+3/4) (-y+1/2,x+3/4,z+1/4) (y+5/8,x+1/8,-z+3/8) (-y+7/8
(x+3/4,z+1/4,-y+1/2) (-x+1/2,z+3/4,y+1/4) (-x,-z,-y) (x+1/4,-z+1/2,y+3/4) (x+5/8,z+1/8,-y+3/8) (-x+3/8
(z+3/4,y+1/4,-x+1/2) (z+1/4,-y+1/2,x+3/4) (-z+1/2,y+3/4,x+1/4) (-z,-y,-x) (z+5/8,y+1/8,-x+3/8) (z+1/8,
(-x,-y,-z) (x+1/4,y+3/4,-z+1/2) (x+3/4,-y+1/2,z+1/4) (-x+1/2,y+1/4,z+3/4) (-x+7/8,-y+7/8,-z+7/8) (x+1/8,

Is there any reason as to why they shift the origin? So, for some cases, the location of the origin is obvious. For others, what happens is there are 2 or more locations where the origin can be placed and usually the origin is placed in some symmetry element. So, if you to address that issue, I will have to go to this materials project web page. And if you go to this, this particular site where you have the various possible space groups for carbon based materials. You go to this Fd 3 bar m, click on that. It shows you it shows you the crystal structure, and here you will have a question mark. You have a question mark right beside the Hermann Mauguin symbol on this webpage.

After I clicked the specific space group that basically opens up a diagram indicating all possible symmetry elements for the diamond structure, which is quite complicated, which is not very easy to read. So, how did I go there? So, I went there like this. So, the materials project page then I have all the structures based on carbon here. So, I know that Fd 3 bar m is what I want to view.

So, I clicked on that and this opens up and then I scroll down and I see the Hermann Mauguin symbol and the corresponding, a question mark right there, I click on that and it opens up this web page. So, the origin here is somewhere here and it is not necessarily placed on an atom always because of Fd 3 bar m is probably the space group for so many different crystals. It is not necessary that it is, so it is for only for carbon, diamond.

And you can have several different possibilities, several different atom types coming up. So, the origin is generally placed at the location of some symmetry elements. So, there are two different choices that are present here, one is at the location of 4, 3 bar m and one other location is at 3 bar, the origin for this.

So, one is called origin choice 1 and other one is called as origin choice 2. The origin choice two which is basically used in the international tables of crystallography but we did not have to know all these things to actually go ahead and construct it. But the origin is generally, no you can read the international tables of crystallography and they will tell you where the origins of are for specific space groups.

So, other things, the reason why I wanted to highlight this diamond structure is that sometimes you will find only two lattice vector or two basis points, but to each of them you will have to add those centering operators in order to get the required multiplicity. So, and whenever you see any center lattices such as a, f, c, i, you find these things on top to which

you will have to add each of these components and after adding make sure that they are not greater than 1 or less than 0, so that you can bring them back into the unit cell, is that clear? Are there any questions you have? Yes.

Student: Could you confidence so high that transformation in, crystallography is greater or not.

(Refer Slide Time: 25:59)

96	h	..2	(y,-y,0) (-y+1/4,-y+1/2,3/4) (y+1/2,y+3/4,1/4) (-y+3/4,y+1/4,1/2) (0,-y,y) (1/4,y+3/4,y+1/2) (3/4,-y+1/2,-y+1/4) (1/2,y+1/4,-y+3/4) (y,0,-y) (y+1/2,1/4,y+3/4) (-y+1/4,3/4,-y+1/2) (-y+3/4,1/2,y+1/4) (-y,y,0) (y+3/4,y+1/2,1/4) (-y+1/2,-y+1/4,3/4) (y+1/4,-y+3/4,1/2)
96	g	..m	(x,x,z) (-x+3/4,-x+1/4,z+1/2) (-x+1/4,x+1/2,-z+3/4) (x+1/2,-x+3/4,-z+1/4) (z,x,x) (z+1/2,-x+3/4,-x+1/4) (-z+3/4,-x+1/4,x+1/2) (-z+1/4,x+1/2,-x+3/4) (x,z,x) (-x+1/4,z+1/2,-x+3/4) (x+1/2,-z+3/4,-x+1/4) (-x+3/4,-z+1/4,x+1/2) (x+3/4,x+1/4,-z+1/2) (-x,-x,-z) (x+1/4,-x+1/2,z+3/4) (-x+1/2,x+3/4,z+1/4) (x+3/4,z+1/4,-x+1/2) (-x+1/2,z+3/4,x+1/4) (-x,-z,-x) (x+1/4,-z+1/2,x+3/4) (z+3/4,x+1/4,-x+1/2) (z+1/4,-x+1/2,x+3/4) (-z+1/2,x+3/4,x+1/4) (-z,-x,-x)
48	f	2.m m	(x,1/8,1/8) (-x+3/4,1/8,5/8) (1/8,x,1/8) (5/8,-x+3/4,1/8) (1/8,1/8,x) (1/8,5/8,-x+3/4) (7/8,x+1/4,3/8) (7/8,-x,7/8) (x+3/4,3/8,3/8) (-x+1/2,7/8,3/8) (7/8,3/8,-x+1/2) (3/8,3/8,x+3/4)
32	e	.3m	(x,x,x) (-x+3/4,-x+1/4,x+1/2) (-x+1/4,x+1/2,-x+3/4) (x+1/2,-x+3/4,-x+1/4) (x+3/4,x+1/4,-x+1/2) (-x,-x,-x) (x+1/4,-x+1/2,x+3/4) (-x+1/2,x+3/4,x+1/4)
16	d	.-3m	(1/2,1/2,1/2) (1/4,3/4,0) (3/4,0,1/4) (0,1/4,3/4)
16	c	.-3m	(0,0,0) (3/4,1/4,1/2) (1/4,1/2,3/4) (1/2,3/4,1/4)
8	b	-43m	(3/8,3/8,3/8) (1/8,5/8,1/8)
8	a	-43m	(1/8,1/8,1/8) (7/8,3/8,3/8)

Wyckoff position and site symmetry group of a specific point

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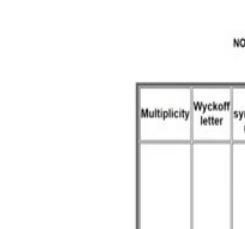

NOTE: *In this table, the representatives of the general positions are transformed as points. (x', y', z') = P⁻¹ (x, y, z).*
Click here to see the transformation of the general position representatives as symmetry operations

Multiplicity	Wyckoff letter	Site symmetry (std.)	Coordinates	
		Standard/Default setting		
		(0,0,0) + (0,1/2,1/2) + (1/2,0,1/2) + (1/2,1/2,0) +		(0,0,0) +
192	i	1	(x,y,z) (-x+3/4,-y+1/4,z+1/2) (-x+1/4,y+1/2,-z+3/4) (x+1/2,-y+3/4,-z+1/4) (z,x,y) (z+1/2,-x+3/4,-y+1/4) (-z+3/4,-x+1/4,y+1/2) (-z+1/4,x+1/2,-y+3/4) (y,z,x) (-y+1/4,z+1/2,-x+3/4) (y+1/2,-z+3/4,-x+1/4) (-y+3/4,-z+1/4,x+1/2) (y+3/4,x+1/4,-z+1/2) (-y,-x,-z) (y+1/4,-x+1/2,z+3/4) (-y+1/2,x+3/4,z+1/4) (x+3/4,z+1/4,-y+1/2) (-x+1/2,z+3/4,y+1/4) (-x,-z,-y) (x+1/4,-z+1/2,y+3/4) (z+3/4,y+1/4,-x+1/2) (z+1/4,-y+1/2,x+3/4) (-z+1/2,y+3/4,x+1/4) (-z,-y,-x) (-x,-y,-z) (x+1/4,y+3/4,-z+1/2) (x+3/4,-y+1/2,z+1/4) (-x+1/2,y+1/4,z+3/4) (-z,-x,-y) (-z+1/2,x+1/4,y+3/4) (z+1/4,x+3/4,-y+1/2) (z+3/4,-x+1/2,y+1/4) (-y,-z,-x) (y+3/4,-z+1/2,x+1/4) (-y+1/2,z+1/4,x+3/4) (y+1/4,z+3/4,-x+1/2) (-y+1/4,-x+3/4,z+1/2) (y,x,z) (-y+3/4,x+1/2,-z+1/4) (y+1/2,-x+1/4,-z+3/4) (-x+1/4,-z+3/4,y+1/2) (x+1/2,-z+1/4,-y+3/4) (x,z,y) (-x+3/4,z+1/2,-y+1/4) (-z+1/4,-y+3/4,x+1/2) (-z+3/4,y+1/2,-x+1/4) (z+1/2,-y+1/4,-x+3/4) (z,y,x)	(x+7/8,y+7/8,z+7/8) (-x+5/8 (z+7/8,x+7/8,y+7/8) (z+3/8, (y+7/8,z+7/8,x+7/8) (-y+1/8 (y+5/8,x+1/8,-z+3/8) (-y+7/8 (x+5/8,z+1/8,-y+3/8) (-x+3/8 (z+5/8,y+1/8,-x+3/8) (z+1/8, (-x+7/8,-y+7/8,-z+7/8) (x+1/8, (-z+7/8,-x+7/8,-y+7/8) (-z+3/8 (-y+7/8,-z+7/8,-x+7/8) (y+5/8, (-y+1/8,-x+5/8,z+3/8) (y+7/8, (-x+1/8,-z+5/8,y+3/8) (x+3/8, (-z+1/8,-y+5/8,x+3/8) (-z+5/8
96	h	..2	(0,y,-y) (3/4,-y+1/4,-y+1/2) (1/4,y+1/2,y+3/4) (1/2,-y+3/4,y+1/4) (-y,0,y) (-y+1/2,3/4,-y+1/4) (y+3/4,1/4,y+1/2) (y+1/4,1/2,-y+3/4) (y,-y,0) (-y+1/4,-y+1/2,3/4) (y+1/2,y+3/4,1/4) (-y+3/4,y+1/4,1/2) (0,-x,x) (1/4,-x+3/4,x+1/2) (3/4,-x+1/2,-x+1/4) (1/2,x+1/4,-x+3/4)	(7/8,y+7/8,-y+7/8) (5/8,-y+1/8 (-y+7/8,7/8,y+7/8) (-y+3/8,5/8 (y+7/8,-y+7/8,7/8) (-y+1/8,-y+ (7/8,-x+7/8,x+7/8) (1/8,x+5/8,

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1/4) (-y+1/2,-y+1/4,3/4) (y+1/4,-y+3/4,1/2)	(-y+7/8,y+7/8,7/8) (y+5/8,y+3/8,1/8) (-y+3/8,-y+1/8,5/8) (y+1/8,-y+5/8,3/8)
-x+3/4,-x+1/4,z+1/2) (-x+1/4,x+1/2,-z+3/4) (x+1/2,-x+3/4,-z+1/4) z+1/2,-x+3/4,-x+1/4) (-z+3/4,-x+1/4,x+1/2) (-z+1/4,x+1/2,-x+3/4) -x+1/4,z+1/2,-x+3/4) (x+1/2,-z+3/4,-x+1/4) (-x+3/4,-z+1/4,x+1/2) -x,-x,-z) (x+1/4,-x+1/2,z+3/4) (-x+1/2,x+3/4,z+1/4) -x+1/2,z+3/4,x+1/4) (-x,-z,-x) (x+1/4,-z+1/2,x+3/4) z+1/4,-x+1/2,x+3/4) (-z+1/2,x+3/4,x+1/4) (-z,-x,-x)	(x+7/8,x+7/8,z+7/8) (-x+5/8,-x+1/8,z+3/8) (-x+1/8,x+3/8,-z+5/8) (z+3/8,-x+5/8,-z+1/8) (z+7/8,x+7/8,y+7/8) (z+3/8,-x+5/8,-x+1/8) (-z+5/8,-x+1/8,x+3/8) (-z+1/8,x+3/8,-x+5/8) (x+7/8,z+7/8,x+7/8) (-x+1/8,z+3/8,-x+5/8) (x+3/8,-z+5/8,-x+1/8) (-x+5/8,-z+1/8,x+3/8) (x+5/8,x+1/8,-z+3/8) (-x+7/8,-x+7/8,-z+7/8) (x+1/8,-x+3/8,z+5/8) (-x+3/8,x+5/8,z+1/8) (x+5/8,z+1/8,-x+3/8) (-x+3/8,z+5/8,x+1/8) (-x+7/8,-z+7/8,-x+7/8) (x+1/8,-z+3/8,x+5/8) (z+5/8,x+1/8,-x+3/8) (z+1/8,-x+3/8,x+5/8) (-z+3/8,x+5/8,x+1/8) (-z+7/8,-x+7/8,-x+7/8)
1,1/8,5/8) (1/8,x,1/8) (5/8,-x+3/4,1/8) '8,-x+3/4) (7/8,x+1/4,3/8) (7/8,-x,7/8) 2,7/8,3/8) (7/8,3/8,-x+1/2) (3/8,3/8,x+3/4)	(x+7/8,0,0) (-x+5/8,0,1/2) (0,x+7/8,0) (1/2,-x+5/8,0) (0,0,x+7/8) (0,1/2,-x+5/8) (3/4,x+1/8,1/4) (3/4,-x+7/8,3/4) (x+5/8,1/4,1/4) (-x+3/8,3/4,1/4) (3/4,1/4,-x+3/8) (1/4,1/4,x+5/8)
-x+3/4,-x+1/4,x+1/2) (-x+1/4,x+1/2,-x+3/4) (x+1/2,-x+3/4,-x+1/4) -x,-x,-x) (x+1/4,-x+1/2,x+3/4) (-x+1/2,x+3/4,x+1/4)	(x+7/8,x+7/8,x+7/8) (-x+5/8,-x+1/8,x+3/8) (-x+1/8,x+3/8,-x+5/8) (x+3/8,-x+5/8,-x+1/8) (x+5/8,x+1/8,-x+3/8) (-x+7/8,-x+7/8,-x+7/8) (x+1/8,-x+3/8,x+5/8) (-x+3/8,x+5/8,x+1/8)
0) (3/4,0,1/4) (0,1/4,3/4)	(3/8,3/8,3/8) (1/8,5/8,7/8) (5/8,7/8,1/8) (7/8,1/8,5/8)
1/4,1/2,3/4) (1/2,3/4,1/4)	(7/8,7/8,7/8) (5/8,1/8,3/8) (1/8,3/8,5/8) (3/8,5/8,1/8)
1/8)	(1/4,1/4,1/4) (0,1/2,0)
3/8)	(0,0,0) (3/4,1/4,1/4)

[Transformation matrix]

For comments, please mail to
administrador.bcs@ehu.eus

NPTEL

ional Setting Help

of the group *Fd-3m* (No. 227) [origin choice 2]

formation matrix (P, p): a,b,c ; 1/8,1/8,1/8

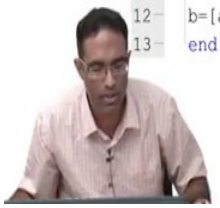
rix form: (P, p) = $\begin{pmatrix} 1 & 0 & 0 & 1/8 \\ 0 & 1 & 0 & 1/8 \\ 0 & 0 & 1 & 1/8 \end{pmatrix}$

ves of the general positions are transformed as points: (x', y', z') = P^{-1} (x, y, z).
rmation of the general position representatives as symmetry operations

Coordinates	
Standard/Default setting	**Transformed**
(0,0,0) + (0,1/2,1/2) + (1/2,0,1/2) + (1/2,1/2,0) +	(0,0,0) + (0,1/2,1/2) + (1/2,0,1/2) + (1/2,1/2,0) +
(-x+3/4,-y+1/4,z+1/2) (-x+1/4,y+1/2,-z+3/4) (x+1/2,-y+3/4,-z+1/4)	(x+7/8,y+7/8,z+7/8) (-x+5/8,-y+1/8,z+3/8) (-x+1/8,y+3/8,-z+5/8) (x+3/8,-y+5/8,-z+1/8
(z+1/2,-x+3/4,-y+1/4) (-z+3/4,-x+1/4,y+1/2) (-z+1/4,x+1/2,-y+3/4)	(z+7/8,x+7/8,y+7/8) (z+3/8,-x+5/8,-y+1/8) (-z+5/8,-x+1/8,y+3/8) (-z+1/8,x+3/8,-y+5/8
(-y+1/4,z+1/2,-x+3/4) (y+1/2,-z+3/4,-x+1/4) (-y+3/4,-z+1/4,x+1/2)	(y+7/8,z+7/8,x+7/8) (-y+1/8,z+3/8,-x+5/8) (y+3/8,-z+5/8,-x+1/8) (-y+5/8,-z+1/8,x+3/8
(-y,-x,-z) (y+1/4,-x+1/2,z+3/4) (-y+1/2,x+3/4,z+1/4)	(y+5/8,x+1/8,-z+3/8) (-y+7/8,-x+7/8,-z+7/8) (y+1/8,-x+3/8,z+5/8) (-y+3/8,x+5/8,z+1/8)
(x+1/2,z+3/4,y+1/4) (-x,-z,-y) (x+1/4,-z+1/2,y+3/4)	(x+5/8,z+1/8,-y+3/8) (-x+3/8,z+5/8,y+1/8) (-x+7/8,-z+7/8,-y+7/8) (x+1/8,-z+3/8,y+5/8)
(+1/4,-y+1/2,x+3/4) (-z+1/2,y+3/4,x+1	1/8,-x+3/8) (z+1/8,-y+3/8,x+5/8) (-z+3/8,y+5/8,x+1/8) (-z+7/8,-y+7/8,-x+7/8
(+1/4,y+3/4,-z+1/2) (x+3/4,-y+1/2,z+1	+7/8,-z+7/8) (x+1/8,y+5/8,-z+3/8) (x+5/8,-y+3/8,z+1/8) (-x+3/8,y+1/8,z+5/8)

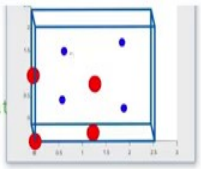
NPTEL

```
1  function [b]= getbasis_diamond()
2  % Given Fd-3m
3   % Positions for 8a. Last number is used to identify the ato
4   A=[0 0 0 1];
5   B=[1/4 1/4 1/4 2];
6   %A=[0 0 0 1];
7   %B=[0.25 0.25 0.25 2];
8
9   a=basis_symm8a(A);%<Get all the basis for this position
10  c=basis_symm8a(B);%< Get all the basis for this postion
11
12  b=[a;c];
13  end
```

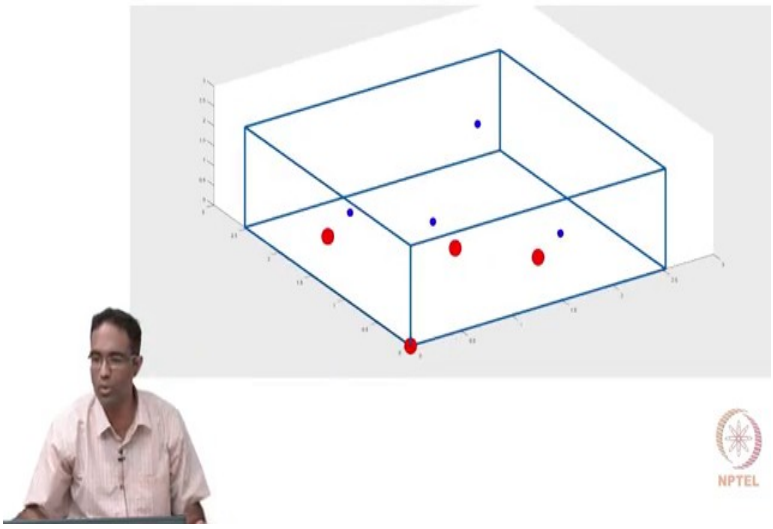


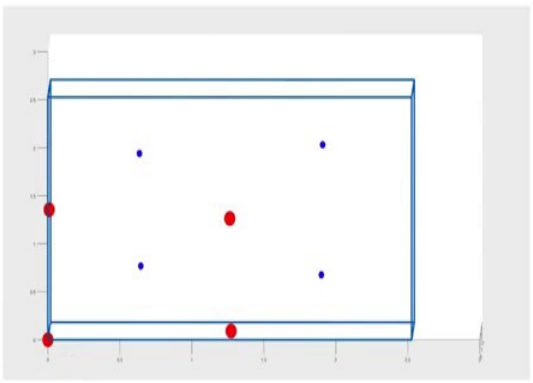
NPTEL

```
31  % b=8.6365;
32  % c=5.1355;
33  % beta=103.98;
34  %Lattice constant
35  %a=4.519;
36  %b=4.519;
37  %c=5.050;
38  %appropriate cell vectors
39  V=[a 0 0;0 b 0; 0 0 c];%Lattice vectors for diamond (Fd-3m
40  %V=[a 0 0;0 b 0; 0 0 c];% Lattice vectors for PdS (P4_2/m)
41  %V=[a 0 0;0 b 0; 0 0 c];% Lattive vectors for (K2MnS2) Iba
42  %V=[a 0 0; 0 b 0; 0 0 c ]; % the three lattice vectors for
43  %V=[a 0 0;0 b 0;c*cosd(beta) 0 c*sind(beta)];% Lattice vec
```



NPTEL





Professor: Sure, I will do that. So, the question is how to apply this transformation, so as to get your basis calculated in some nonstandard setting. So, let us go back, so we click Fd 3 bar m. And then when you click standard default setting, you will get what I got previously where the, this is what you would get, and you will find the atom at 1 by 8, 1 by 8, 1 by 8, 7 by 8, 3 by 8, 3 by 8. Now I want to shift, I want to make this 0, 0, 0, the I want the origin to be located right on top of the atom. So, what I do here is, I go back and click non-conventional setting.

And it tells me what sort of transformation I want to apply. So, this is basically a linear transformation, you can rotate it, you can rotate the origin and all that. You can rotate the coordinate system and all that. We do not need that we just need a origin shift. So, I am going to shift it by 1 by 8, 1 over 8, 1 over 8 and then click change the basis. And then it gives me

on the left hand column, the standard default setting and on the right hand column, it gives me the transformed the thing, where 1 by 8, 1 by 8, 1 by 8 becomes 0, 0, 0. And basically 1 by 8, 1 by 8, 1 by 8 has been subtracted from all the various basis.

Student: diamond cubic has 1 by 4, 1 by 4, 1 by 4, but here 3 by 4, 1 by 4, 1 by 4 in site??

Professor: 3 by 4, diamond cubic is 1 by 4, 1 by 4, 1 by 4, there is an atom at 1 by 4, 1 by 4, 1 by 4 and you are telling me that here it is 3 by 4, 1 by 4, 1 by 4, you put 1 by 4, 1 by 4, 1 by 4 or 3 by, because when you add this half here, all these things will, it will automatically generate that 1 by 4, 1 by 4, 1 by 4 that you are talking about. So, it does not matter.

So, I go here. I go to my get basis command instead of 0, 0, 0, 1, okay 0, 0, 0, 1, quarter, quarter, quarter, 2 and if I click run, it generates a structure you look at look at how the atoms are oriented, it is oriented with 2 atoms this way, 2 atoms that way and then the corresponding face centered atoms here.

These are all the face centrics, is the right? Now, if I just change it, it is just the only thing that has happened, it has been rotated this way. There is no other difference, from crystalographically there is no other difference. Is that right? Are you able to see that, yes or no?

Student: Yes.

Student: Sir, this in this, in this if we observe the corner atom at the left and then we see that next here, the blue is the atom which will be near to the left back . But in the case, it is some right.

Professor: so will there be , there will be atom here, no? Which will now ...

It is down, the other one is up.

Professor: This one. So, will there be but there will be an atom here now, which will now, which it is down, so it is up, yes.

Student: The other alternating void will start coming

Professor: The other alternative voids will start coming, so you this is actually the diamond structure. If you put 3 by 4, 3 by 4, 3 by 4 is what you get the actual diamond structure. They look the same but I think the directions are a little bit different. So, in one you would have an

atom at quarter, quarter, quarter but when you repeat it, see for example, that this one is at quarter, quarter, quarter with respect to this, this corner atom. If I put a red atom right here, which is going to exist, that this one will be at the quarter, quarter, quarter, it will be down, it will be down.

Now, this direction and this direction are they going to be the same for diamond cubic structures? The 111 and 1 bar, 1, 1, you will have to think about it. They both may not necessarily be equivalent. Is that answer your question?

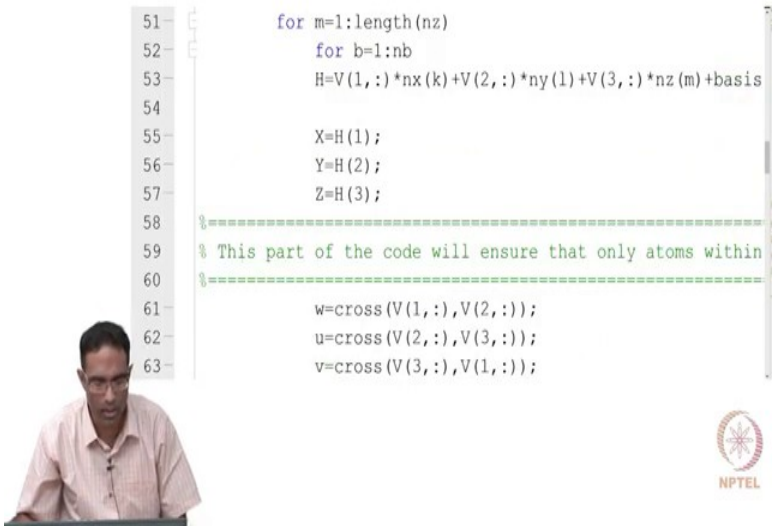
Student: Yeah, I wanted to know the difference, you know if it is 1 by 4, 1 by 4, 1 by 4 or 3 by 4, 3 by 4, 3 by 4 they may give the same symmetry?

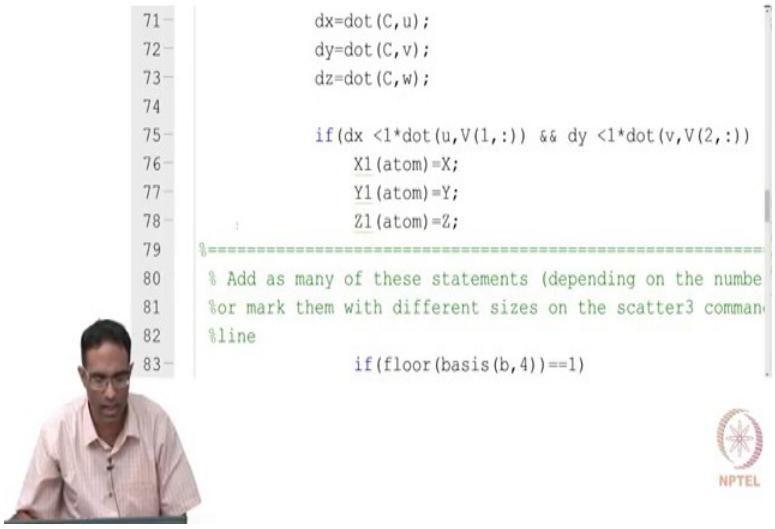
Professor: They are not, they give the same symmetry, yes because you have generated from the same symmetry system only. We like to work it out completely to actually take a look, so we will see that later. What is that?

Student: It might become enantiomorphous pairs of each other.

Professor: But, in this there is no real 4, 1 or 4, 4 to actually have enantiomorphous pairs. It is not the enantiomorphous, it just depends on how it is being transformed and rotated. I think you, I believe you can transform and rotate either one to make them coincide. That is what I think. You have to give it a shot.

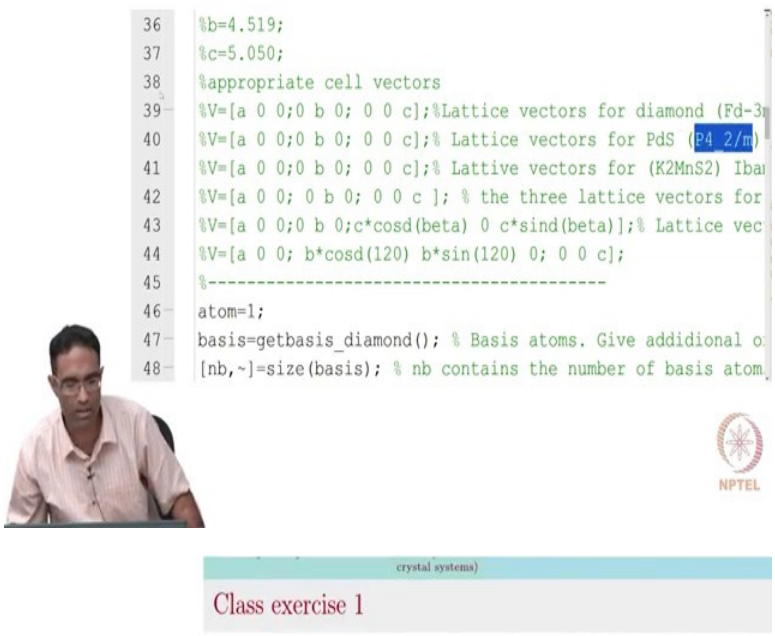
(Refer Slide Time: 31:48)

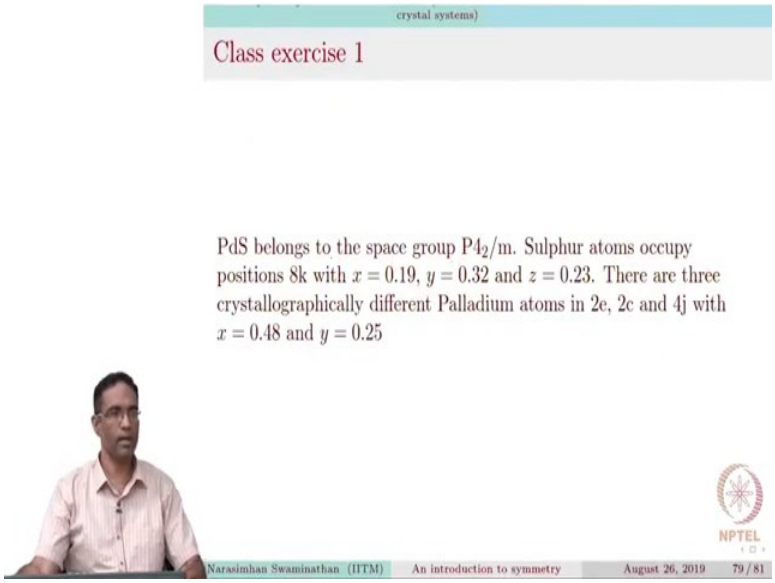




How would I restrict to one unit cell? So there is, there are there are commands that are present in the main MATLAB program. That is between line numbers 61 to 78 which will essentially take care of that. It is based on some analytical geometry which I assume you will find out how it works. But if you do this, it will work, anything else? Nothing else, okay good.

(Refer Slide Time: 32:26)

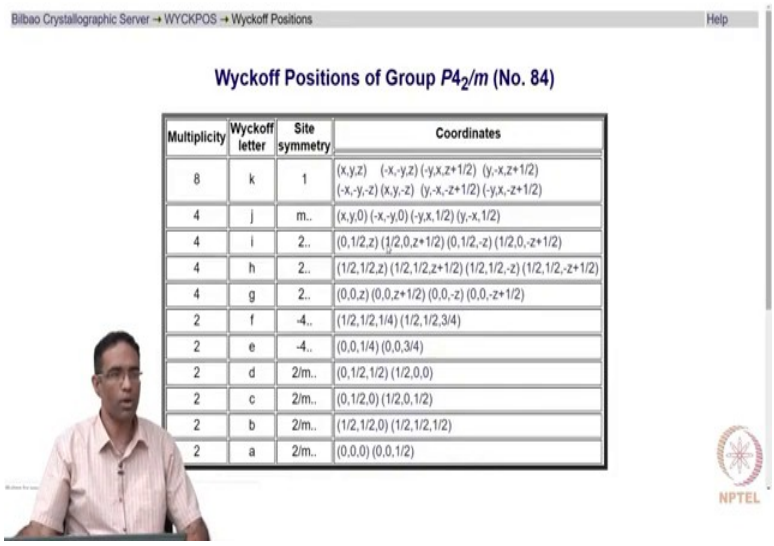




So, let us go to the next structure that we want to create. So, I want to create PdS, Palladius sulphide as we call it. And it has the space group 4, 2 over m, this is a space group for Palladius sulphide. And like what we discussed yesterday, so P 4, 2 means it is basically a tetragonal unit cell. And like what we discussed yesterday, there is there are sulphur atoms which occupy 8k positions with axis 0.19 and y as 0.32 and z as 0.23 and there are 3 cryptographically different palladium atoms at 2e, 2c and 4j positions. Once you specify 4j, you also have to give the corresponding fractional x and the fractional y coordinate.

(Refer Slide Time: 33:28)

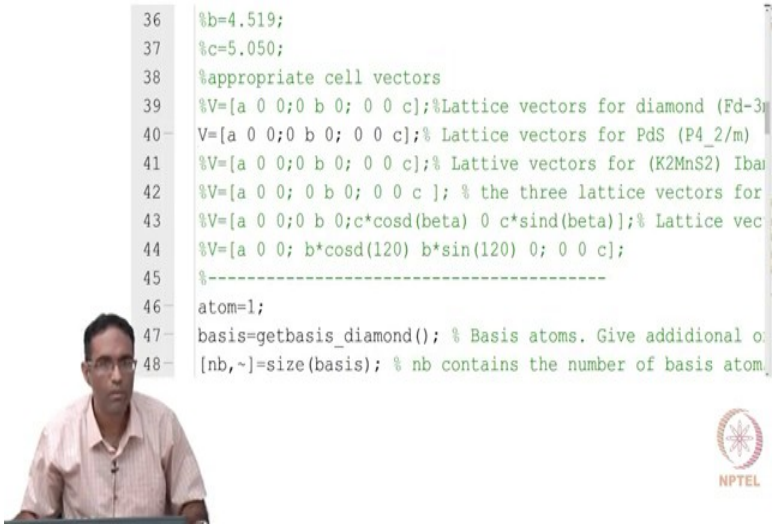
81	$P\bar{4}$	82	$I\bar{4}$	83	$P4/m$	84	$P4_2/m$	85	$P4/n$
86	$P4_2/n$	87	$I4/m$	88	$I4_1/a$	89	$P422$	90	$P42_12$
91	$P4_122$	92	$P4_12_12$	93	$P4_222$	94	$P4_22_12$	95	$P4_322$
96	$P4_32_12$	97	$I422$	98	$I4_122$	99	$P4mm$	100	$P4bm$
101	$P4_2cm$	102	$P4_2nm$	103	$P4cc$	104	$P4nc$	105	$P4_2mc$
106	$P4_2bc$	107	$I4mm$	108	$I4cm$	109	$I4_1md$	110	$I4_1cd$
111	$P\bar{4}2m$	112	$P\bar{4}2c$	113	$P\bar{4}2_1m$	114	$P\bar{4}2_1c$	115	$P\bar{4}m2$
116	$P\bar{4}c2$	117	$P\bar{4}b2$	118	$P\bar{4}n2$	119	$I\bar{4}m2$	120	$I\bar{4}c2$
121	$I\bar{4}2m$	122	$I\bar{4}2d$	123	$P4/mmm$	124	$P4/mcc$	125	$P4/nbm$
126	$P4/nnc$	127	$P4/mbm$	128	$P4/mnc$	129	$P4/nmm$	130	$P4/ncc$
131	$P4_2/mmc$	132	$P4_2/mcm$	133	$P4_2/nbc$	134	$P4_2/nnm$	135	$P4_2/mbc$
136	$P4_2/mnm$	137	$P4_2/nmc$	138	$P4_2/ncm$	139	$I4/mmm$	140	$I4/mcm$
141	$I4_1/amd$	142	$I4_1/acd$	143	$P3$	144	$P3_1$	145	$P3_2$
146	$R3$	147	$P\bar{3}$	148	$R\bar{3}$	149	$P312$	150	$P321$
151	$P3_112$	152	$P3_121$	153	$P3_212$	154	$P3_221$	155	$R32$
156	$P3m1$	157	$P31m$	158	$P3c1$	159	$P31c$	160	$R3m$
161	$R3c$	162	$P\bar{3}1m$	163	$P\bar{3}1c$	164	$P\bar{3}m1$	165	$P\bar{3}c1$
166	$R\bar{3}m$	167	$R\bar{3}c$	168	$P6$	169	$P6_1$	170	$P6_5$



Bilbao Crystallographic Server → WYCKPOS → Wyckoff Positions Help

Wyckoff Positions of Group $P4_2/m$ (No. 84)

Multiplicity	Wyckoff letter	Site symmetry	Coordinates
8	k	1	(x,y,z) (-x,-y,z) (-y,x,z+1/2) (y,-x,z+1/2) (-x,-y,-z) (x,y,-z) (y,-x,-z+1/2) (-y,x,-z+1/2)
4	j	m..	(x,y,0) (-x,-y,0) (-y,x,1/2) (y,-x,1/2)
4	i	2..	(0,1/2,z) (1/2,0,z+1/2) (0,1/2,-z) (1/2,0,-z+1/2)
4	h	2..	(1/2,1/2,z) (1/2,1/2,z+1/2) (1/2,1/2,-z) (1/2,1/2,-z+1/2)
4	g	2..	(0,0,z) (0,0,z+1/2) (0,0,-z) (0,0,-z+1/2)
2	f	-4..	(1/2,1/2,1/4) (1/2,1/2,3/4)
2	e	-4..	(0,0,1/4) (0,0,3/4)
2	d	2/m..	(0,1/2,1/2) (1/2,0,0)
2	c	2/m..	(0,1/2,0) (1/2,0,1/2)
2	b	2/m..	(1/2,1/2,0) (1/2,1/2,1/2)
2	a	2/m..	(0,0,0) (0,0,1/2)



```
36  %b=4.519;
37  %c=5.050;
38  %appropriate cell vectors
39  %V=[a 0 0;0 b 0; 0 0 c];%Lattice vectors for diamond (Fd-3
40  V=[a 0 0;0 b 0; 0 0 c];% Lattice vectors for PdS (P4_2/m)
41  %V=[a 0 0;0 b 0; 0 0 c];% Lattive vectors for (K2MnS2) Iba
42  %V=[a 0 0; 0 b 0; 0 0 c ]; % the three lattice vectors for
43  %V=[a 0 0;0 b 0;c*cosd(beta) 0 c*sind(beta)];% Lattice vec
44  %V=[a 0 0; b*cosd(120) b*sin(120) 0; 0 0 c];
45  %----------------------------------------
46  atom=1;
47  basis=getbasis_diamond(); % Basis atoms. Give addidional o
48  [nb,~]=size(basis); % nb contains the number of basis atom
```

So, we go to our crystallographic web page P4, 2 over m, 84, right? Standard or default setting, in standard or default setting whenever you talk about orthorhombic space groups, the B axis is going to be horizontal, the axis will be vertically pointing downwards and you will be looking at it through the from the C axis. So, which is essentially saying that A axis is horizontal, B axis vertically pointing up and C axis pointing outside the plane of the paper, the simple, not confusing at all system that has been used for the structure.

So, there is a point called 8k and these are the various points that you will have to generate x, y, z, minus x, minus y, z and so on, so 1, 2, 3, 4, 5, 6, 7, 8 points. So, let us see how those 8 points are being generated?

Student: What you just told now, this is horizontal, this is vertical, what does that matter?

Professor: Well, if you in the international tables of crystallography, if you take a look at, how does this vertical or horizontal way of organizing your a, b, c vectors a matter? So, in international tables of crystallography, which we do not discuss here in detail, you do not have 3 dimensional diagrams, you have 2 dimensional diagrams. And you can actually specify x, y, z with respect to the x normally whenever we talk about the fractional x coordinate, we are always associating it with a and normal y coordinate, we are associating it with b and c with the z coordinate.

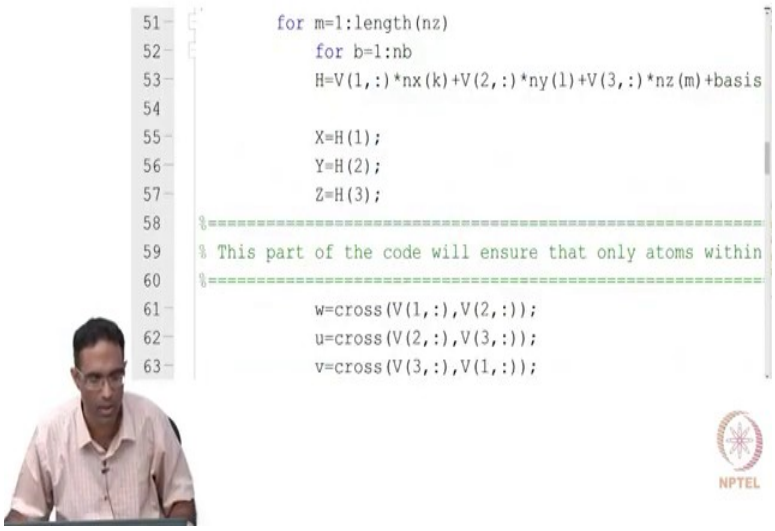
But I could very well choose a system which is not that way, I could draw this as c, this as a and this is b. And you have to be careful to choose your x, y and z fraction coordinate accordingly. So, whenever we when you see in the international tables of crystallography, you would see a b vector going pointing out to the right, a vector pointing to the bottom and automatically to mean that the c vector is pointing outside, Ok? And which is the same as a horizontal, b vertical and c vector pointed to the outside.

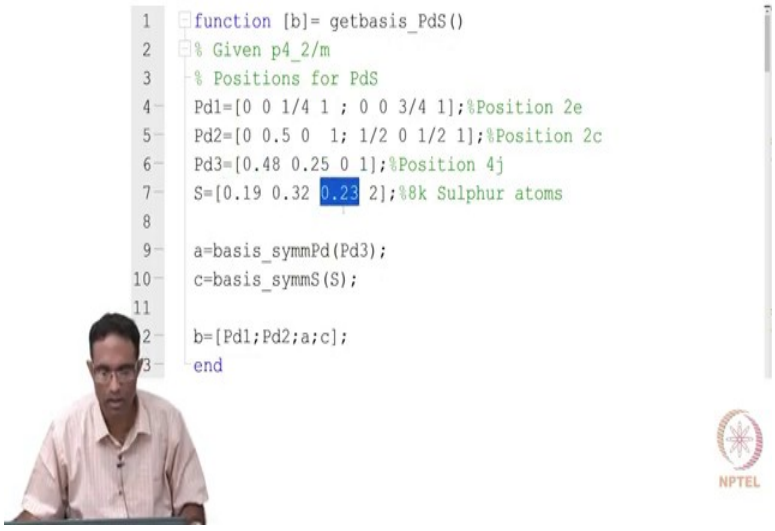
It is also possible to have a coordinate system where you have, where you look at it from the b axis for example, in the mean mono clinical lattice. Whenever we are talking about the mono clinic lattice they would say that the b axis is unique. What that means is? This is a, this is c and this would be b or the b would be the axis which has a 2 fold coordination number. In that case, you would have to associate the y with this b and not with the c. It will make a difference in the final structure that you generate. We will, I think I have an example showing that we will see when it comes.

Student: Sir you said that the outward pointing vector is the highest symmetry.

Professor: Usually the outward pointing vector will have the highest symmetry or will be called as a unique axis. The b axis is the unique axis in the mono clinic structure, they will tell you, b axis,… unique b axis.

(Refer Slide Time: 36:49)





Wyckoff Positions of Group $P4_2/m$ (No. 84)

Multiplicity	Wyckoff letter	Site symmetry	Coordinates
8	k	1	(x,y,z) (-x,-y,z) (y,-x,z+1/2) (-y,x,z+1/2) (-x,-y,-z) (x,y,-z) (y,-x,-z+1/2) (-y,x,-z+1/2)
4	j	m..	(x,y,0) (-x,-y,0) (-y,x,1/2) (y,-x,1/2)
4	i	2..	(0,1/2,z) (1/2,0,z+1/2) (0,1/2,-z) (1/2,0,-z+1/2)
4	h	2..	(1/2,1/2,z) (1/2,1/2,z+1/2) (1/2,1/2,-z) (1/2,1/2,-z+1/2)
4	g	2..	(0,0,z) (0,0,z+1/2) (0,0,-z) (0,0,-z+1/2)
2	f	-4..	(1/2,1/2,1/4) (1/2,1/2,3/4)
2	e	-4..	(0,0,1/4) (0,0,3/4)
2	d	2/m..	(0,1/2,1/2) (1/2,0,0)
2	c	2/m..	(0,1/2,0) (1/2,0,1/2)
2	b	2/m..	(1/2,1/2,0) (1/2,1/2,1/2)
2	a	2/m..	(0,0,0) (0,0,1/2)

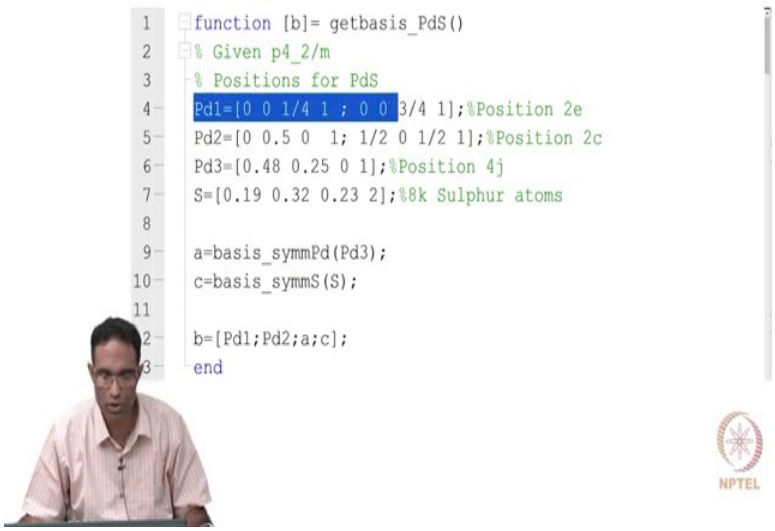

```
z=X(3);

basisa(1,1:3)=[x y z];
basisa(2,1:3)=[-x -y z];
basisa(3,1:3)=[-y x z+0.5];
basisa(4,1:3)=[y -x z+0.5];
basisa(5,1:3)=[-x -y -z];
basisa(6,1:3)=[x y -z];
basisa(7,1:3)=[y -x -z+0.5];
basisa(8,1:3)=[-y x -z+0.5];
```


```
for j = 1:8
    for k=1:3
 if(basisa(j,k) < 0)
     basisa(j,k)=1-abs(basisa(j,k));
 end
     if(basisa(j,k) > 1)
    basisa(j,k)=abs(basisa(j,k))-1;
end
end
    end
end
```

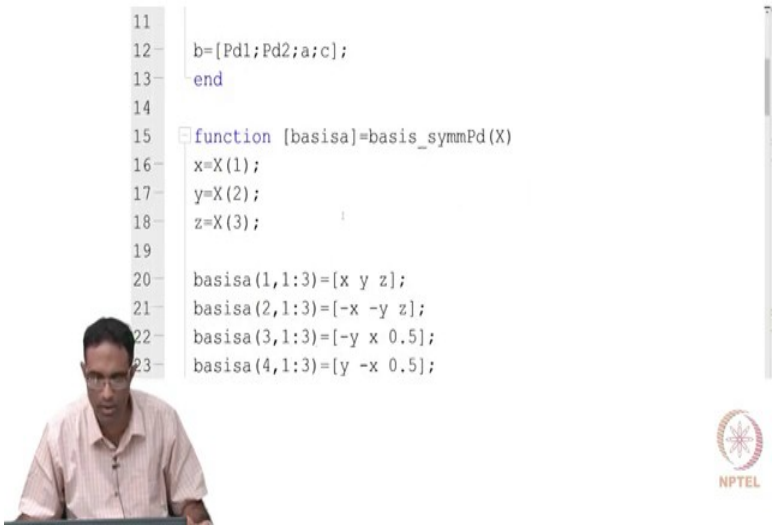
I think I have a example there, we will see that it is not PdS though, PdS is quite straightforward. So, in PDS we have one 8k position. So, let us open that PdS, I did not give this to you, so you do not have it with you. So, I just want to want you to follow right here. So, in PdS, the sulphur is present at 8k position and these are the 3 values. So, I have named a sulphur atom with atom type 2 the x fractional coordinate, y fractional coordinate and z fractional coordinate are given right here.

And for 8k, there are 1, 2, 3, 4, 5, 6, 7, 8, 8 additional points that I need to generate. Therefore, I have basis underscore sym S sub function right here, where I will generate all of them. And I will also make sure that the fourth column is the same as x4, which is the same type and I will go over all these atom x, y, z fractional coordinates and pull them all inside the unit cell by either subtracting them from 1 or adding minus 1 to these particular coordinates to actually pull them back into the unit cell.

(Refer Slide Time: 38:01)



Multiplicity	Wyckoff letter	Site symmetry	Coordinates
8	k	1	(x,y,z) (-x,-y,z) (-y,x,z+1/2) (y,-x,z+1/2) (-x,-y,-z) (x,y,-z) (y,-x,-z+1/2) (-y,x,-z+1/2)
4	j	m..	(x,y,0) (-x,-y,0) (-y,x,1/2) (y,-x,1/2)
4	i	2..	(0,1/2,z) (1/2,0,z+1/2) (0,1/2,-z) (1/2,0,-z+1/2)
4	h	2..	(1/2,1/2,z) (1/2,1/2,z+1/2) (1/2,1/2,-z) (1/2,1/2,-z+1/2)
4	g	2..	(0,0,z) (0,0,z+1/2) (0,0,-z) (0,0,-z+1/2)
2	f	-4..	(1/2,1/2,1/4) (1/2,1/2,3/4)
2	e	-4..	(0,0,1/4) (0,0,3/4)
2	d	2/m..	(0,1/2,1/2) (1/2,0,0)
2	c	2/m..	(0,1/2,0) (1/2,0,1/2)
2	b	2/m..	(1/2,1/2,0) (1/2,1/2,1/2)
2	a	2/m..	(0,0,0) (0,0,1/2)



Now, I have to do this for the other atoms as well. So, one Pd, the other Pd 1, the palladium first atom is actually present at 0, 0, quarter, 1, 0, 0, 3 by 4, 1. So, I can either give them like this or in the form of 2 separate rows like we had in the diamond structure and I go over all these atoms, so Pd 1 just has 2 points. Just this right, 2, b, is that right? Is it 2, b, it is 2, b, so half, half, 0, half, half, half. 2 e was 0, 0, quarter, 0, 0, 3 by 4. So, 0, 0, quarter, 0, 0, 3 by 4 are just given directly. Pd 2 has a position 2 c, 0.50 and half, 0, half which can also be seen here in position 2 c, these two.

Then I have Pd 3 which is presented a position 4j for which the x coordinate is 0.48 and the y coordinate is 0.25 and the z coordinate is 0. However, position 4j requires some additional points to be generated because of the symmetry. So, 4j right here, so it is x, y,0, minus x,

minus y, 0, minus y, x, half, y, minus, x half, There is a negative there are negative things coming in, so I like have to make sure that I am pulling them all back inside the unit cell.

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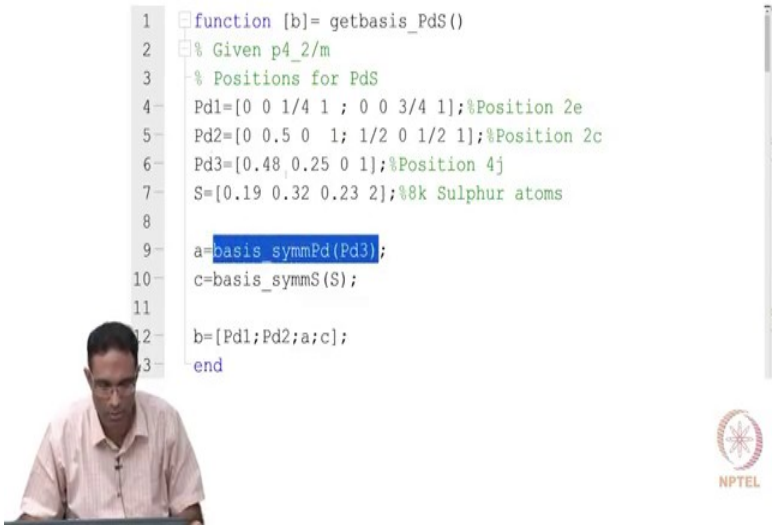

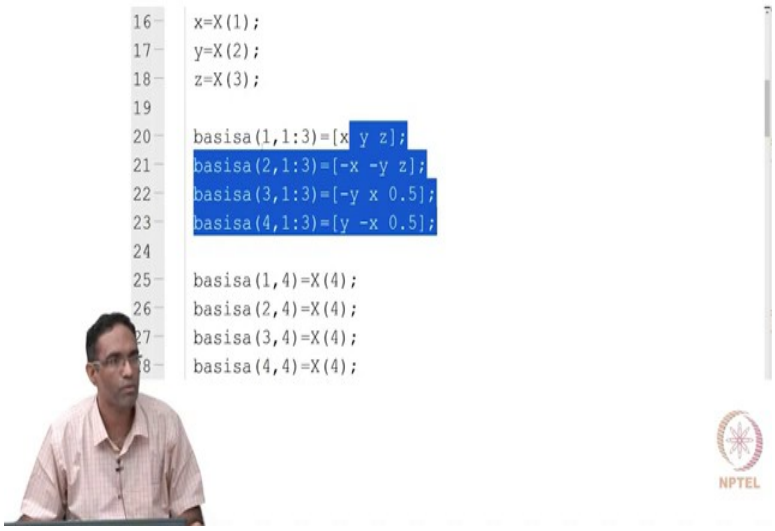

So, I write another small function basis symm Pd and give this Pd 3 alone to it, which will basically generate all the necessary points for that particular Pd. So, now if you see the total number of atoms inside the unit cell is going to be 2 plus 2 plus this is 4, 2 plus 2, 4, 4 plus 4, 8, 8 plus 8, 16. There are 16 atoms that is present inside one unit sell of PdS.

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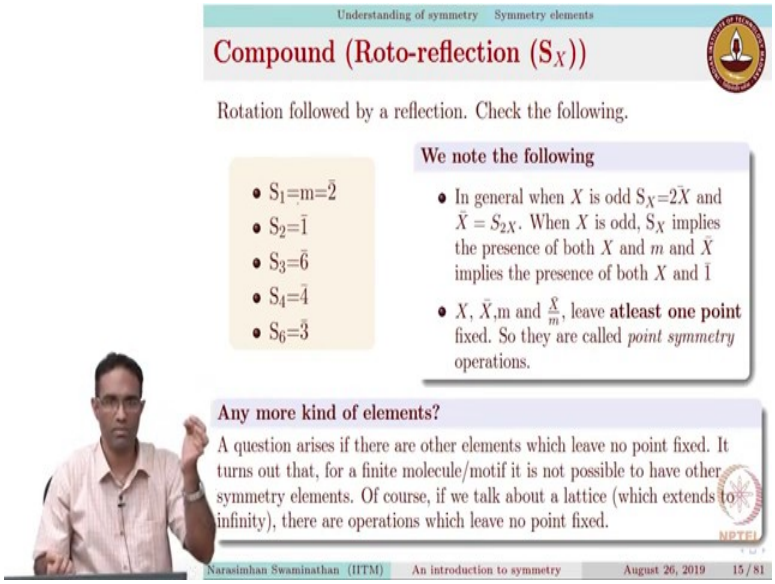

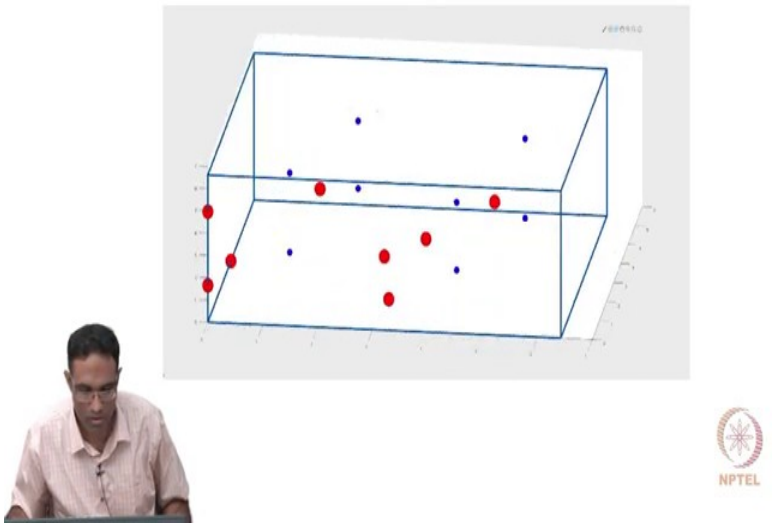

So, we go back here to the main program. We do not have to change much here. We just have to change choose appropriate lattice constants and choose the appropriate lattice vector. That is this one right here, sorry you remind me, so I need to change the get basis command to be that of PdS and that is the crystal structure for PdS.

So, these are the, I think the palladium atoms and the other ones are probably the sulphur atoms. So, this is how you generate the structure. Of course, it is important for us to know whether we generated it correctly. So, it is a good idea to actually go to our materials project website.

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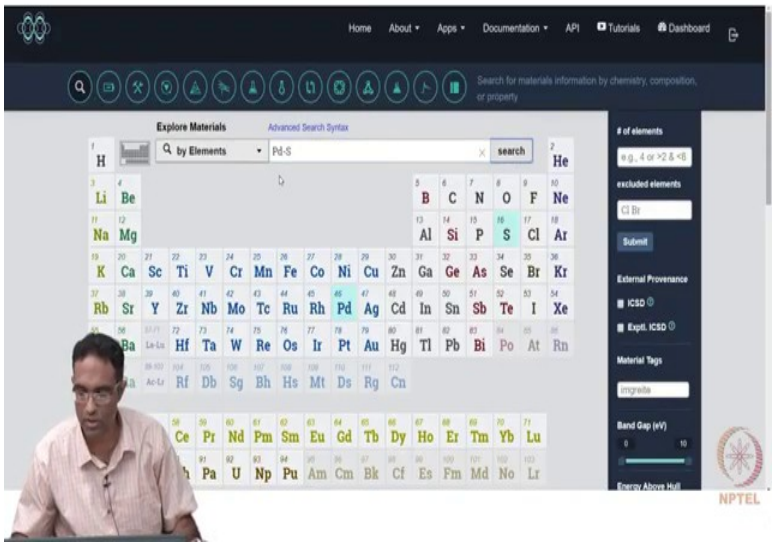
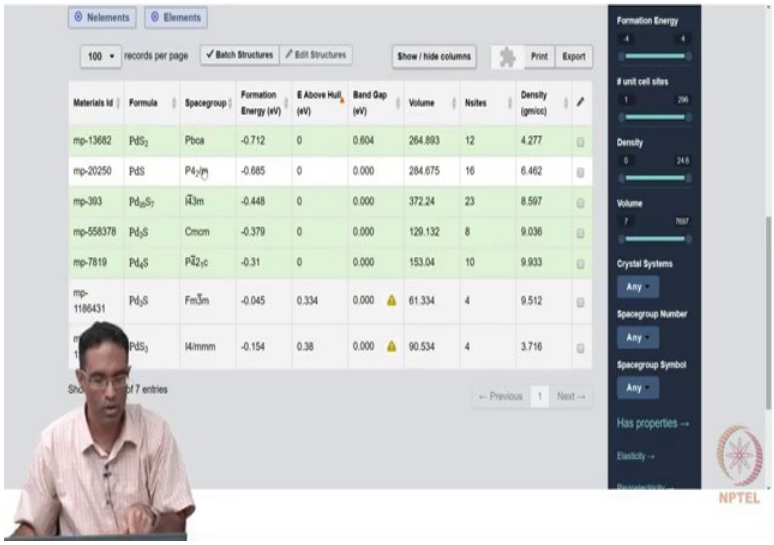
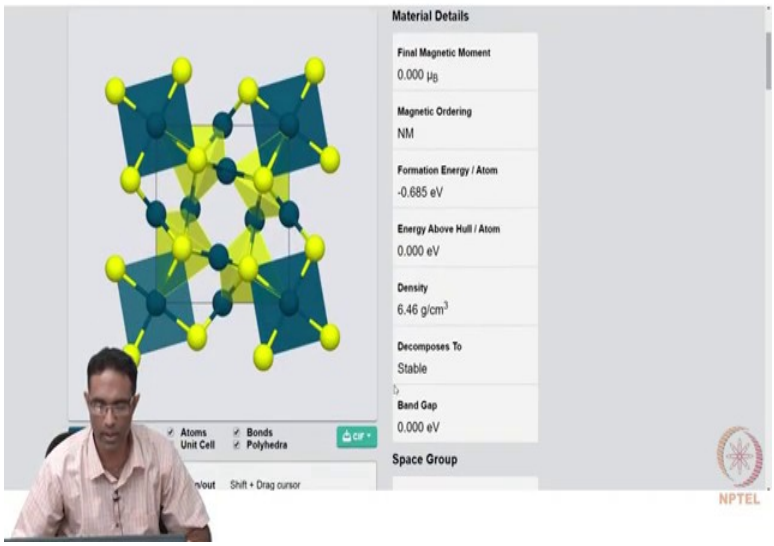
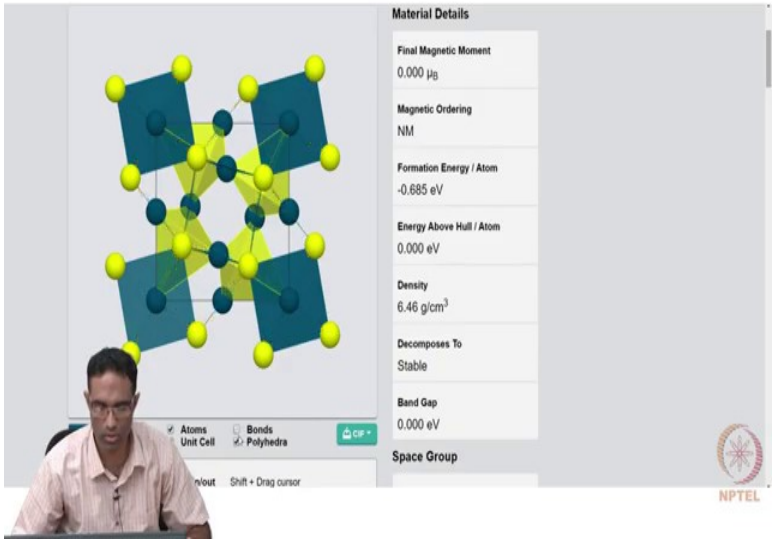
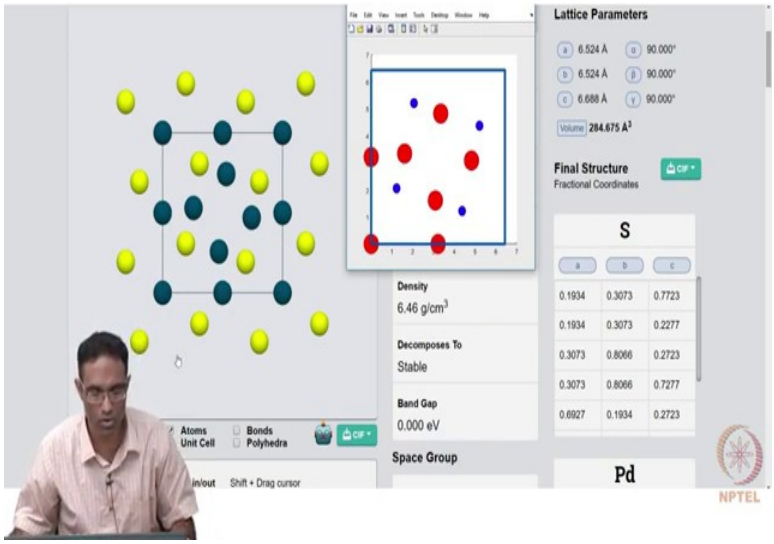







Material Details
Final Magnetic Moment
0.000 μ_B
Magnetic Ordering
NM
Formation Energy / Atom
-0.685 eV
Energy Above Hull / Atom
0.000 eV
Density
6.46 g/cm^3
Decomposes To
Stable
Band Gap
0.000 eV
Space Group
Atoms
Bonds
Unit Cell
Polyhedra
CIF
Shift + Drag cursor
NPTEL


Lattice Parameters
a 6.524 Å
α 90.000°
b 6.524 Å
β 90.000°
c 6.688 Å
γ 90.000°
Volume 284.675 Å^3
Final Structure
Fractional Coordinates
CIF
S
a b c
0.1934 0.3073 0.7723
0.1934 0.3073 0.2277
0.3073 0.8066 0.2723
0.3073 0.8066 0.7277
0.6927 0.1934 0.2723
Density
6.46 g/cm^3
Decomposes To
Stable
Band Gap
0.000 eV
Space Group
Pd
Atoms
Bonds
Unit Cell
Polyhedra
Shift + Drag cursor
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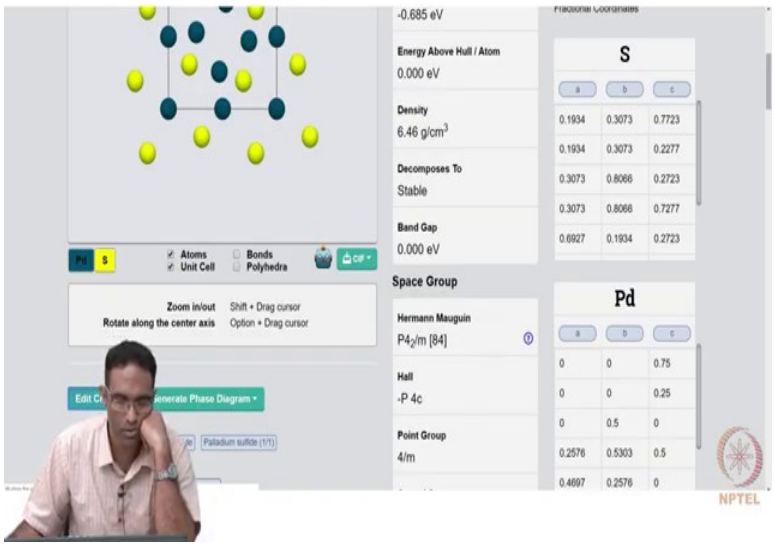
-0.685 eV
Energy Above Hull / Atom
0.000 eV
Density
6.46 g/cm^3
Decomposes To
Stable
Band Gap
0.000 eV
Space Group
S
a b c
0.1934 0.3073 0.7723
0.1934 0.3073 0.2277
0.3073 0.8066 0.2723
0.3073 0.8066 0.7277
0.6927 0.1934 0.2723
Pd
Atoms
Bonds
Unit Cell
Polyhedra
CIF
Zoom in/out
Shift + Drag cursor
Rotate along the center axis
Option + Drag cursor
Hermann Mauguin
$P4_2/m$ [84]
Hall
-P 4c
Point Group
4/m
Generate Phase Diagram
Palladium sulfide (1/1)
0 0 0.75
0 0 0.25
0 0.5 0
0.2576 0.5303 0.5
0.4697 0.2576 0
NPTEL

Choose PdS, search, so PdS 4 2 over m is what we generated. So, we click on that, just take some time. So, in this manner, you can actually generate almost all the structures that you need. It is very simple. Now, this looks very complicated here. So, I just remove the bonds, I remove the polyhedral. So, you see all these things, all these atoms, so this is the palladium atom. This is, is it looking like the way we generated? Can we convince ourselves that you have generated it correctly?

Yes? So this, this one is right here, this one right here, this one is right here. And then you have these 4 atoms appearing here and then the sulphur atoms right here. It looks a little bit skewed because MATLAB is not plotting it correctly. Otherwise it should be. It should look squarish. You are looking it from the C axis.

And again if you want to, so that is PdS. So, the PdS is pretty simple. It is not very complicated, but you can see how the structure can get pretty complicated if you have larger number of atoms per unit cell. You should know how to check in through this website.

Student: Sir, the translations with system conserved ?

Professor: What is, what did you say translation of the?

Student: Translation of symmetry is conserved here.

Professor: Conserved, here in this in this website thing, they have also plotted the those atoms, so if you did not want to take a look at it, you just need to click edit crystal and then uncheck repeat atoms and the periodic boundary conditions and you would say exactly only

those atoms contained within the unit cell, which we can see if it opens up, the problem with the subset is just taking a little bit longer. So, that is PdS for you.

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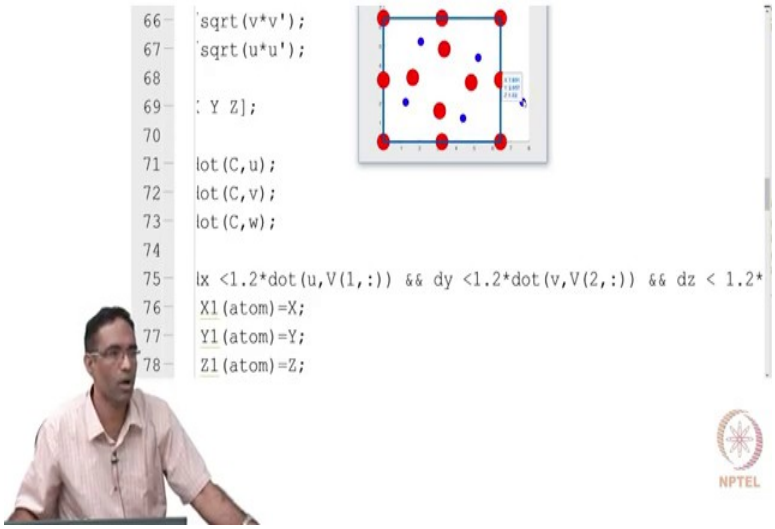

Now, we can of course, extend this a little bit like I showed you, you can actually print all the atoms that is a little bit more than one unit cell, maybe by saying 1.2. Now, it is a little bit more than one unit cell has been printed. You can put 1.1 and you will make sure that you can make sure that these 2 atoms are actually not going to get printed. Are there any questions for this aspect? I know you may not have enough time to actually code it right now and see you can do it later on in your at home. So, but this is just a demonstration for the space group P4, 2 over m. Question yeah?

Student: From this generic site why it is not so many position .

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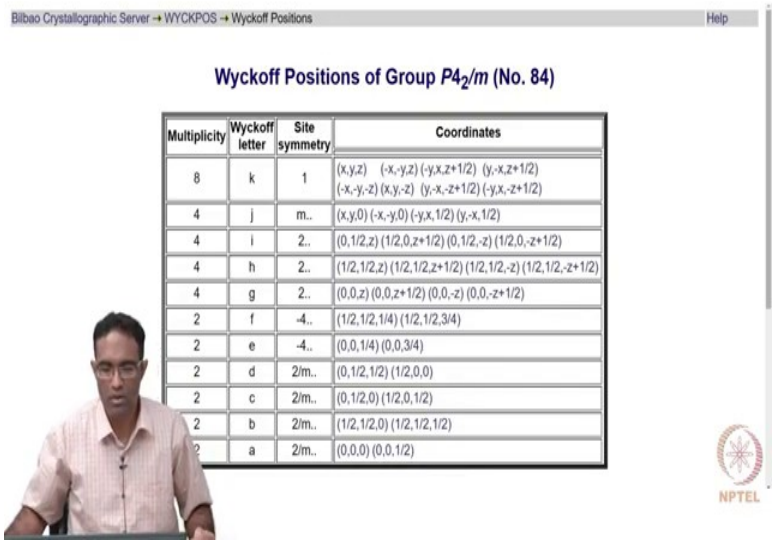

Professor: For the generic site means you mean this one, this one this one.

Student: No, the other one there it is showing all the sites and its coordinates

Professor: This one? Why does it have 8 sites? Because see P4, 2 or m, what does it mean? It means that this is a tetragonal space group, but it is, first of all P4 itself will generate 4. But now what you are doing is, you have 4 fold rotation and you have another perpendicular to it. So, there is a 4 fold rotation. It is not just a 4 fold rotations, screw axis, you are performing a 4 fold rotation and moving it half the unit cell and there is a mirror just perpendicular to it.

So, the set of all these operations that will be generated that will be applied on one generic point x, y, z will generate these additional points. This is exactly what we did for P4, the simple case.

Student: How will we get the coordinates and what is the site symmetry

Professor: Site symmetry is one. So, the question is what is the site symmetry? Site symmetry means, it is a general point, the particular point is not lying over any symmetry element. That is what it means, if it starts to lie over a symmetry element, the multiplicity reduces. For example, the point 4j the multiplicities and that means that point lies on a mirror, it lies on x, y, 0 or z is equal to half, it lies on a mirror.

Once the point starts lying on a symmetry element, the number of additional points that get generated by applying all symmetry elements that is appropriate for the space group P4 2

over m will be lower than what you get for a point that is not lying on a symmetry element like a general position.

Again The generation of this will involve these matrices, we talked about for P4 remember we use a simple matrix and I too showed you how these points are generated. For this space group also, there are a couple of different matrices that you can generate and study and apply it to a general x, y, z point and generate all these additional points, so it is just possible. But we are just not doing it in this course. That is not our goal because people have done that and given these tables to us. We want to know how to use them, how to use them to generate our structures?

So, first you tell me what is, I explain what is meant by P 4 2 over m. So first question is, what is that? P4 2 over m is a space group. It is one of the space groups or the 230 space groups is one of the space groups. P4 2 over m is basically the Hermann Mauguin's symbol for a space group. And in this particular space group, the symmetry elements that have been applied is a 4 fold rotation, but not just a mere 4 fold rotation. But after applying the 4 fold rotation, I have to move it up along the C axis by half the unit cell.

Not only that, I also should make sure that there is a mirror that is perpendicular to it. All these symmetry elements are there in that space group by m.. means there is a mirror that is perpendicular to the axis that contains the 4 fold rotation. P2 over m means there is a mirror that is perpendicular to the axis that is the, that contains a 2 fold rotation. That is what it means.

Student: One slot, is there 4 2 over m is one slot.

Professor: Yes, exactly 4 2, 4 suffix 2 over m is present in one slot. It refers to just the C axis. That is it. Or in other words, if you want to be precise, it is p 1, 1, 4 suffix 2 over m. But this 1, 1 do not mean anything. So, we just write it as P 4 suffix 2 over m. Is that okay?

Student: Sir, we read about compound symmetry operations in the past, there was a operation roto-reflection in which we came after the symbol S 2, S 4 means rotation followed by a mirror, so if S 2, the same as 2 by m.

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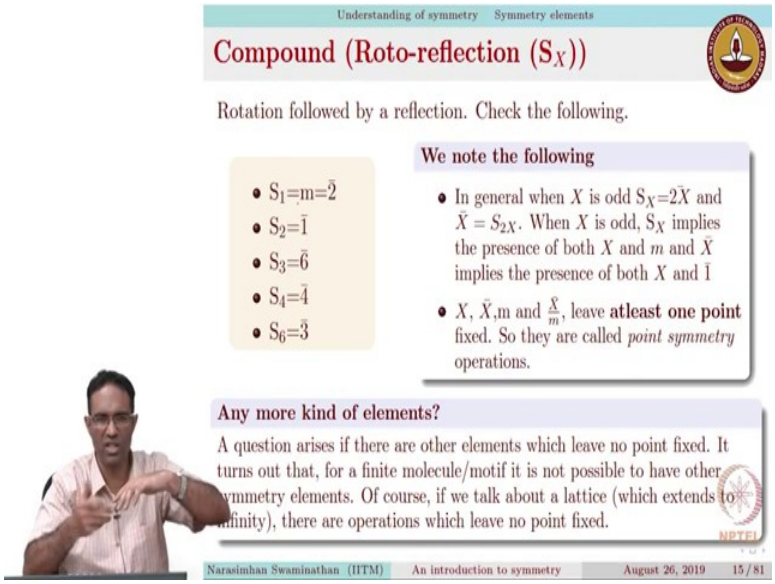

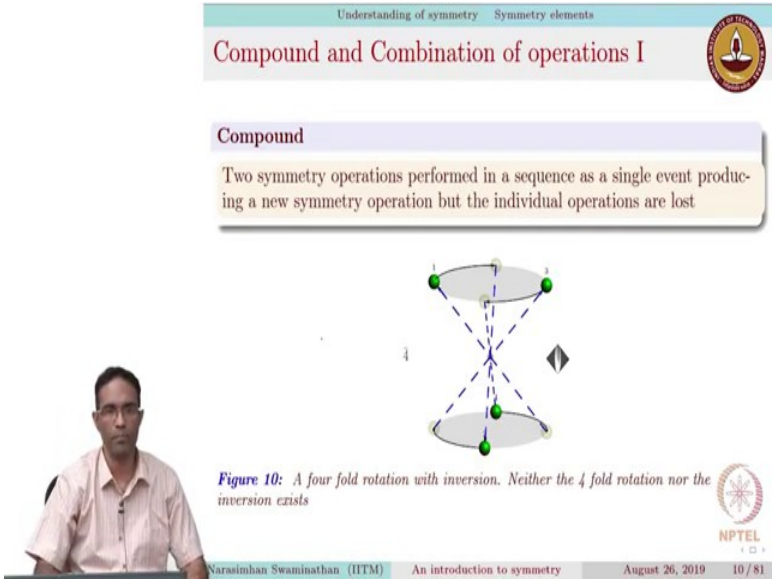

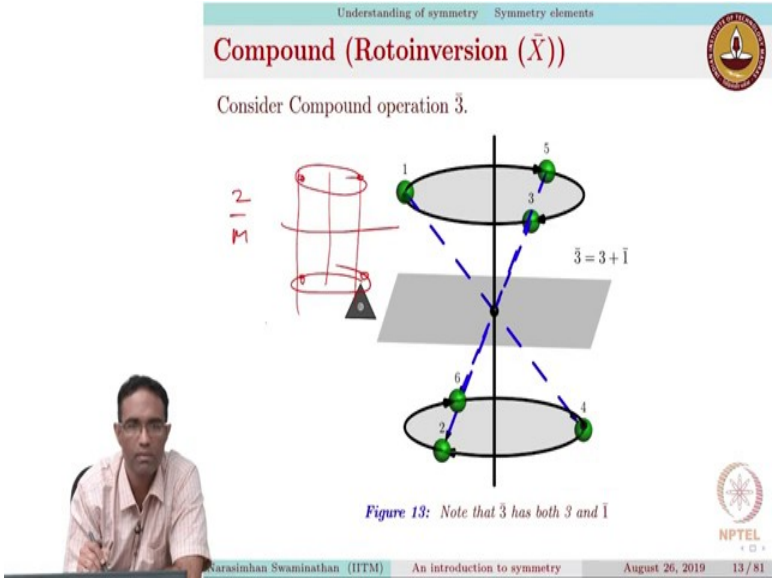

Professor: Is S 2, we studied another set of symbols called as roto reflection and is S 2 the same as 2 over m. I will show you that slide S 2 is 2 fold rotation followed by a mirror. So, it means an inversion, it means an inversion, not a mirror, it is not to… 2 fold rotation, perpendicular to it, there is a mirror, it is just 2 fold rotation.

Student: But is the mirror perpendicular to that 2 fold rotation axis?

Professor: Yes, always, if I write 2 over m, it means that the symmetry elements that are present are a 2 fold rotation and a mirror that is perpendicular to it.

Student: In S 2 also that is the…

Professor: No, S 2 means a 2 fold rotation and a mirror not end a mirror sorry 2 fold rotation and then you apply a mirror operation to it. So, this atom is not there, S 2 means, I have applied the 2 fold rotation and then I applied a mirror. So, this intermediate point is not generated, 2 over m means, the 2 fold rotation is also present and the mirror is also present.

Student: Not audible…

Professor: Yes, if I say 4 suffix 2 over m, it means there is a 4 fold rotation and screw and the translation by about half the unit cell by half the unit cell. And there is also a mirror perpendicular to it. So, it is not.

Student: Sir, taking 2 by m, both 2 and m are independently existing.

Professor: Yes, they will exist. Yes.

Student: But in S 2, they are not independently existing.

Professor: Correct.

Student: They are only present as a combination.

Professor: Correct. That is what happens in say 4 bar say for example 4 bar 4 fold rotation and an inversion, individually 4 and 1 bar is not existing. They are not, for example, if you look at the screen, individually 4 and 1 bar is not existing, 4 bar together, both have to be applied consecutively to generate that operation.

Student: But even in case of S 2 when we apply the 2 fold rotation, they must be applying it about an axis, so the mirror is it perpendicular to that axis, the mirror plane?

Professor: Yes.

Student: It is.

Professor: It is perpendicular to that axis. So, in S 2, it is 2 fold rotation mirror this intermediate point is not generated. In fact, S 2 is therefore just one bar. But, if I say 2 over m, it means there is a 2 fold rotation and there is a mirror perpendicular to it. So, consequently the in 2 over m, you will have this. There is a 2 fold rotation and a mirror that is perpendicular to it. Are there any other questions here? Is okay?

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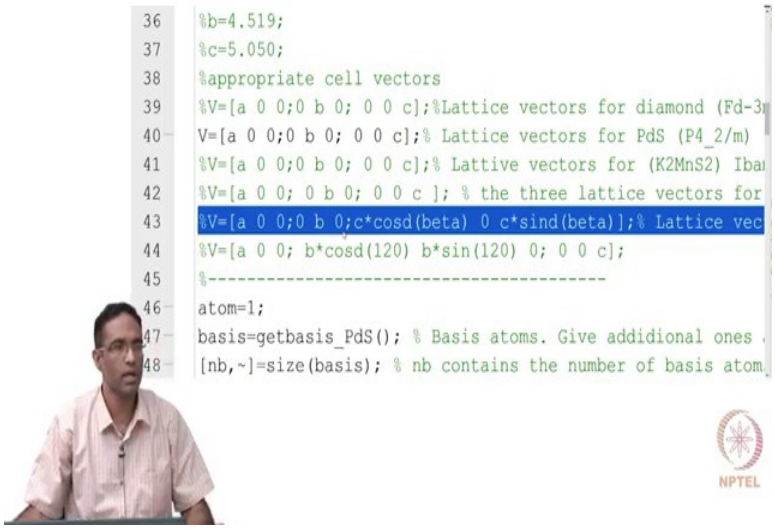

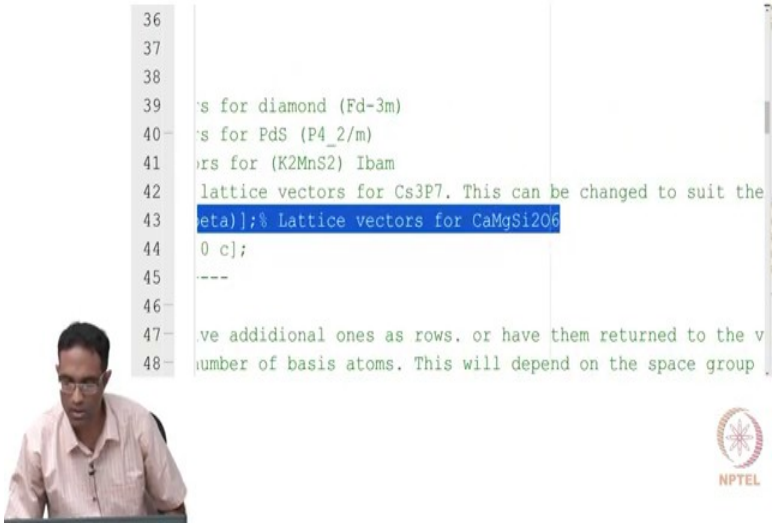

So, we have a couple of more examples. In particular, I think I wanted to talk about this one which is $CaMgSi_2O_6$, which is where a little bit of confusion comes with regards to how you choose your a axis, b axis and z axis. We will do that in the next class.