Foundation of Computational Material Modelling
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Generating 2D crystal with MATLAB using Bilbao Crystallography website

Good afternoon. So, what we were looking at last class is basically the various equivalent positions that can be taken up by a general point when you perform a certain symmetry operation on it and we took the example of the space group p4.

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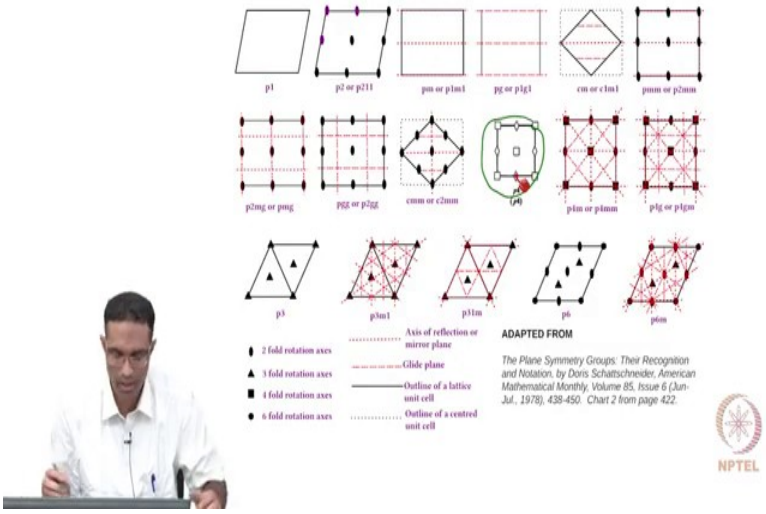

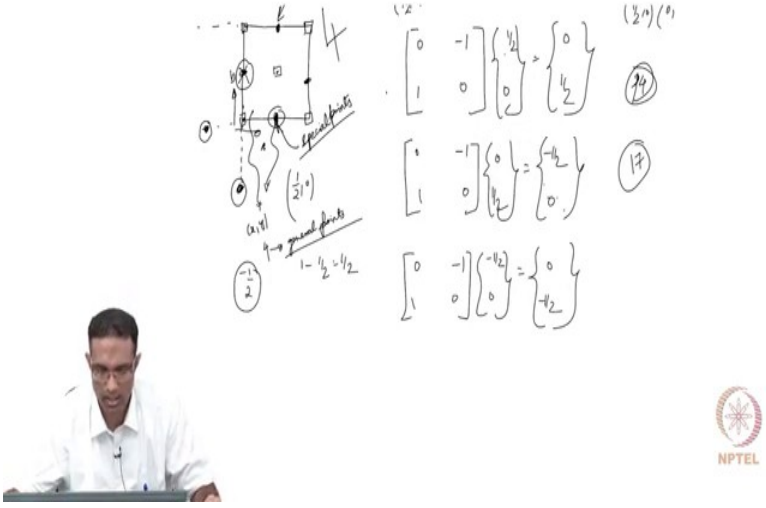

So, let me take you back to the slide which has the list of all space groups here, all the 17 plain groups not the space groups, the plain groups in 2D and we were looking at essentially this one. And when we said that we looked at a certain general point, we essentially meant a point somewhere here and arbitrary point that looked that was present somewhere there? And we performed the P4 operations or the 4 fold rotation operation on that particular point and we got how many points, we got 4 different points they were all equivalent by that symmetry operation that is a 4 fold rotation.

And I mentioned that such points are called as general points, where as there are points, if there is a point which lies on the symmetry element, then you would reduce the total number of multiplicity that is actually possible. So, if you take a look at this p4, so this is the p4 plain group if you have a point right there, then the question it lies on the symmetry element as soon as you have P4 it essentially automatically generates additional two fold rotation axis at this point this point and this point. The presence of the four folds symmetry automatically entails these additional symmetry.

Now if you have a atom that is laying right here what is the fractional coordinate of that point, what is the fractional coordinate of that point? So, if you have this to be b and this to be a, you have the two fold rotation right here here here here and there is a 4 fold. So, the fractional coordinate of this point is half 0. The question is how many new points are going to be generated when we perform the 4 fold rotation? So, we shall start doing one by one so we have half comma 0 given to us and the corresponding rotation matrix or the transformation matrix as you might call it for the 4 fold rotation is this.

We saw this in the last class as well so I am going to multiply it by half and 0 and what do I get? You get half and half I think the rotation matrix is wrong because the four fold rotation cannot be producing half and half, what is rotation matrix for this case?

Student: 0 minus 1.

Professor: 0 minus 1, 1, 0, so half 0 will generate what, first 0 it generated a 0 half. Now you perform a 4 fold rotation on 0 half. Minus half and 0, now we do one more time. So, a good question is to see whether these points are actually different apart.

So, you got this is 1 so you started with half comma 0 and you got a 0 comma half. Then you got minus half comma 0, and then you got another one which is 0 comma minus half. So, with respect to this unit cell right here, this the one that we just started off this one. Where are the other points located, so half comma 0 was located here, 0 comma half is probably located is right here. X is equal to 0 and y is equal to half. Then x is minus half and y is 0 is located right here, correct. And X is equal to 0 and y is equal to minus half is located here. So, if you perform like I told you, if you have minus half you can automatically bring it back into the cell by performing the operation 1 minus half which will give you half. Consequently this point and this point are basically the same points similarly this point and this point are basically the same points.

So, these two points which are being generated by the 4 fold rotation are already there with you, you are just regenerating them. Therefore because this particular point and this is happening simply because this point in lying on the symmetry element that is present there. So this such points are called as special points. Points where you have maximum multiplicity such as a general point here which has a multiplicity of 4 are called as general points. So, when you have a point at half, half, half, if you keep applying 1 0 minus 1 1 0 transformation to it over and over again you are going to generate the same point. Similarly if you have a point at 000 you will keep generating the same point over and over again you will not generate any new points. Therefore the multiplicity of these points is less.

So, this was done for the space group p4, so now there are 17 space groups, each one having a different hormone model symbols and different set of symmetry operations that are basically possible. And it is possible for us to take a general point in each case, for example if you take this particular space group then or a plain group it is possible for us to choose the general points somewhere here and apply p4 and m. you have to apply the 4 fold rotation and the 2 mirrors that is associated with it. And for each and every such operation you have matrix operations such you can do, which is not required for this class. How every you need to know that you know there are mathematical operations which can give you the other points that have been generated because of the symmetry.

And there are also special points such as these points marked by the diamond which indicate a 2 fold rotation and also mirrors. A point could lie on a mirror and if it lies on a mirror it will start generating fewer points than what we did when the point is lying at a general position. So, for

every such plain group there are specific points called general points where you have maximum multiplicity and then you have several special points depending upon the symmetry element on which the point is lying, you will generate a certain number of other points by applying that particular symmetry operator.

And it is important for us to know what these other points are only then we can actually have all the atoms that we know in order to recreate the entire 2 dimensional crystal in this case. So, it so happens that it is not required for us to actually generate these points by hand, they have already been generated and given to us in the form of cryptographic tables, for each and every plain group.

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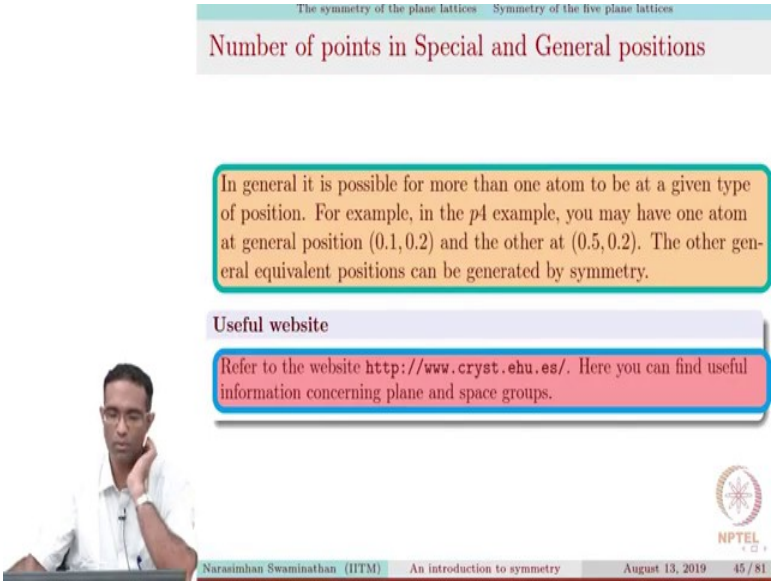


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Representations and Applications
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Subperiodic Groups: Layer, Rod and Frieze Groups
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Raman and Hyper-Raman scattering
Point-group symmetry
Plane-group symmetry
DENPOS
WYCKPOS
MAXSUB
Double point and space groups
Space access to some tables
Space Groups
Plane Groups
Layer Groups
Rod Groups
Frieze Groups
2D Point Groups
3D Point Groups
Magnetic Space Groups
For comments, please mail
NPTEL


Wyckoff Positions of Plane Groups
How to select the group
Please, enter the sequential number of group as given in International Tables for Crystallography, Vol. A or
Choose #
Standard/Default Setting
[Bilbao Crystallographic Server Main Menu]


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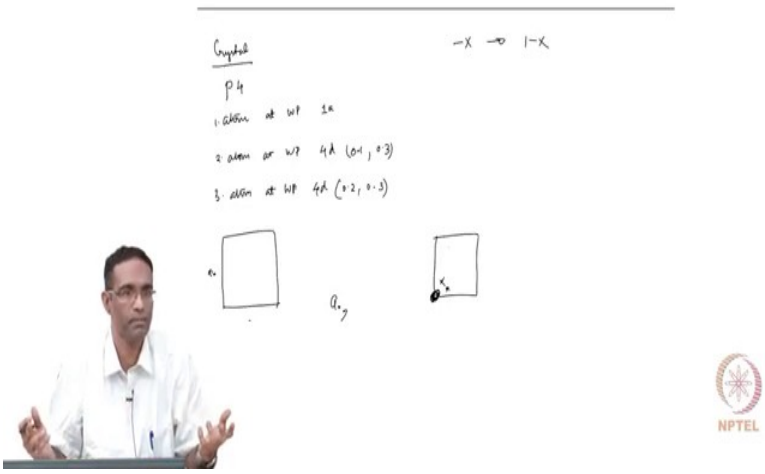
Table of Group Symbols

No plane group has been selected by now

1	p 1
2	p 2
3	p 1 m 1
4	p 1 g 1
5	c 1 m 1
6	p 2 m m
7	p 2 m g
8	p 2 g g
9	c 2 m m
10	p 4
11	p 4 m m
12	p 4 g m
13	p 3
14	p 3 m 1
15	p 3 1 m
16	p 6
17	p 6 m m

Wyckoff Positions of Plane Group p 4 (No. 10)

Mult.	Letter	Site Sym	Coordinates
4	d	1	(0,0) (-x, -y) (-y, x)
2	c	2	(1/2, 1/2) (0, 1/2)
1	b	4	(1/2, 1/2)
1	a	4	(0, 0)



So, this is what we are going to look at a little bit today, so we covered all the stuff so another important point is that in general it is point for more than one atom to actually be located at any general point. So, for example in p4 you could have one general point at 0.2 0.3 and another general point could be located at point 1 0.2 and you have to apply all the symmetry operators appropriate for the particular plain group to that point to generate all the other points inside the unit cell. But that is the sometime the conversion process depending upon the plain group or the space group that you are dealing with and consequently people have already done this because it is just based on these matrix type operations. People have already done this and tabulated it in a nice form which you can actually look at. So, the website that you can refer to is given right here. So, I am gonna click on it and show you little bit of that. So, this is a very useful website you can get a lot of information from this website. So there is something about space groups, space groups deals with 3 dimensional arrangement of atoms and lattice points.

So, we not going to look into that for the purpose of this course we would like to look at space group later on. And then now we are dealing with plain groups so we shall talk a little bit about plain group. So, we are interested in this link which says plain group symmetry, the various positions that are essentially there in which the atoms can be located are called as Wyckoff positions. If you want to look at any one particular plain group understand what are the various Wyckoff positions possible for the particular plain group then you go to the website in the same manner that I just did and then you can click choose it, to choose the Wyckoff position that you

want, choose the plain group for which you want to look at the Wyckoff position and the one that we were looking at is this p4.

So, I am clicking on it and you get a nice table and they tell you several things here, they tell you that this is the plain group p4 and they tell you in the first column something called as mult which is basically the multiplicity of a general point, there is a letter that is associated with each and every position, it starts from a from the lower most row then there is something called site symmetry, that means if there is a symmetry element passing through that point then the symmetry of that side or general side has no symmetry passing though it which is why you create maximum multiplicity consequently its side symmetry is 1 and if you are given x comma y the other points that are going to be generated are minus x, minus y, minus yx, y minus x and I told you how we can actually generate that in a simple manner.

Now if you look at two c the position c to dot dot, that means there is a 2 fold symmetry axis that is passing through that point. So, there are only two different points that you could generate by applying all the symmetry elements associated with the plain group p4 and you got half 00 half and then there are two others one is half half and 00 which is Wyckoff position given by 1 b and 1 a. In general whenever you want to create a crystal or whenever you are looking at a literature or a paper and they want to specify a crystal what they will do is, so whenever you want to create a crystal what will be given to you is that you will be told that the crystal belongs to a specific plain group or space group and you will be said that there is an atom at Wyckoff position say 1a, another atom at Wyckoff position 4d and there will be the corresponding fractional coordinates associated with it. And a third atom again at Wyckoff position 4d but now with a different set of fractional coordinates.

In addition to that since it is a crystal unit the corresponding lattice is constant to actually create this entire crystal. So, once you know the lattice constant, the Wyckoff positions of the atoms constituting that crystal it is possible for you to generate that crystal because what you will do? You will go to this website and you will that there is one atom at 1a so there is an atom at 0 comma 0. So, you will that there is an atom right here then you will also know that there is an atom at 4b, there is one atom at 4d with a specific x and the y value and another atom with a different x comma y value.

But you know that for each x comma y value you are able to generate 4 additional points within the unit cell. So, for this atom you will generate 4 additional points and for this atom also you will generate four additional points. So you know all the atoms that are going to lie inside the unit cell so whenever you see minus x all you have to do is, do one minus x and replace it with one minus x. If you see minus y you have to replace it with one minus y. Then you know all the points lying inside the unit cell and once you know all the atoms laying the unit cell, you can actually generate the entire crystal.

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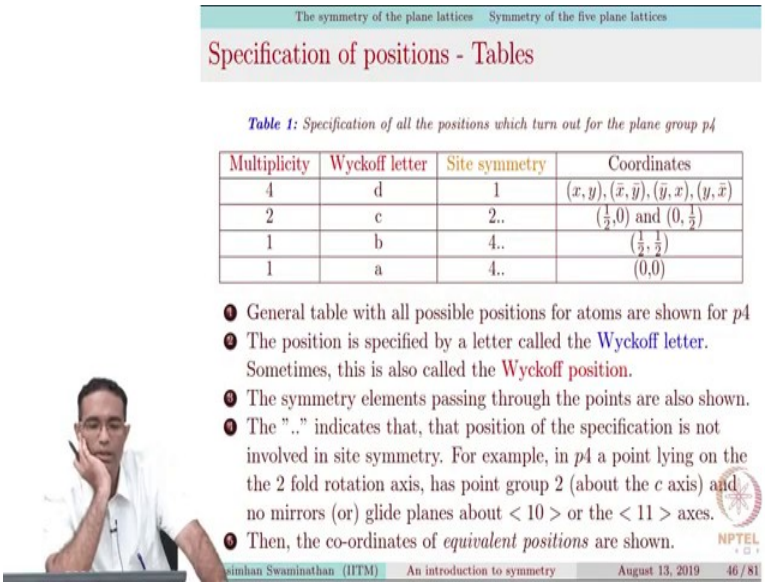
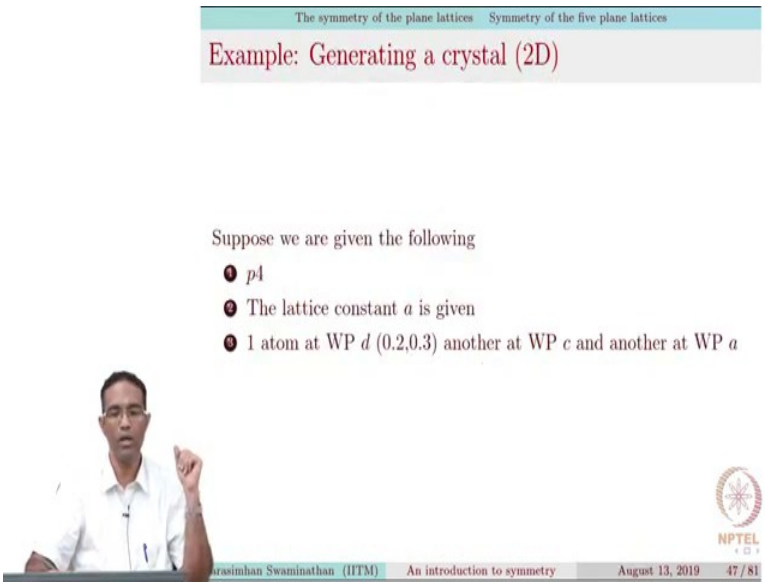




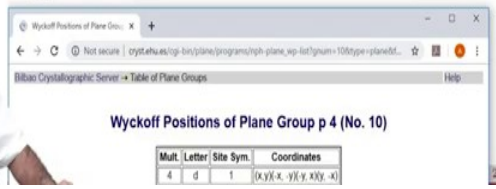
The Code

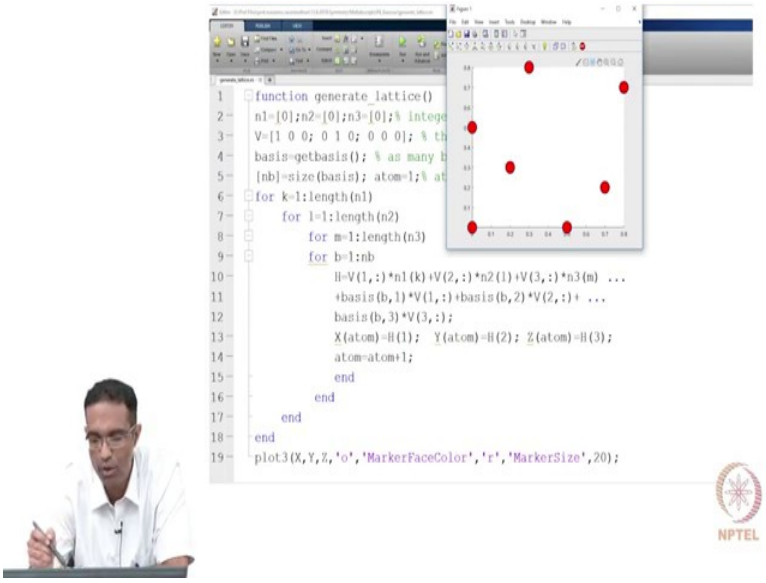
```
function generate_lattice()
n1=[0];n2=[0];n3=[0];% integers
V=[1 0 0; 0 1 0; 0 0 0]; % three lattice vectors (a=1).
basis=getbasis(); % as many basis as needed
[nb]=size(basis); atom=1;% atom is just a counter
for k=1:length(n1)
    for l=1:length(n2)
        for m=1:length(n3)
        for b=1:nb
            H=V(1,:)*n1(k)+V(2,:)*n2(l)+V(3,:)*n3(m) ...
            +basis(b,1)*V(1,:)+basis(b,2)*V(2,:)+ ...
            basis(b,3)*V(3,:);
            X(atom)=H(1);  Y(atom)=H(2); Z(atom)=H(3);
            atom=atom+1;
            end
        end
    end
end
plot3(X,Y,Z,'o','MarkerFaceColor','r','MarkerSize',20);
```

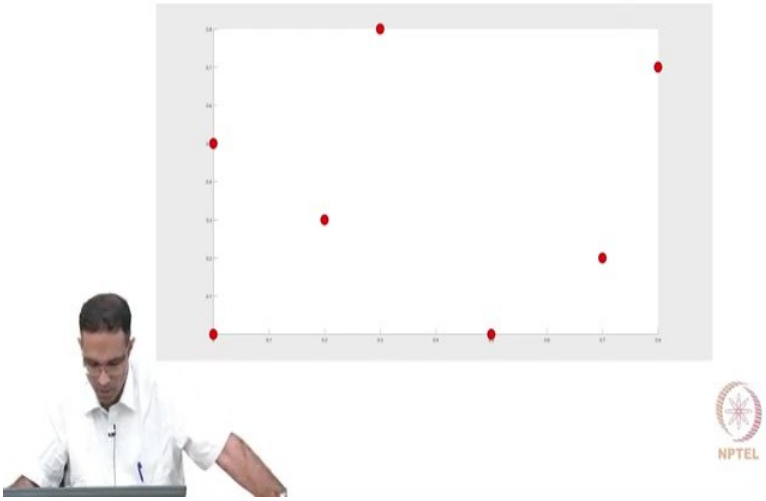
The Code

(0.2, 0.3)

```
function [b]= getbasis()
% Given p4 and that the basis atoms are present at
%WP d, c and a
bd=[0.2 0.3 0;1-0.2 1-0.3 0;1-0.3 0.2 0;0.3 1-0.2 0];
bc=[0.5 0 0; 0 0.5 0];
ba=[0 0 0];
b=[bd ;bc ;ba];
end
```







So, we will see an example of this right now so this is the p4 plain group and I have just regenerated that table right here, you can also look at it in the website, I just taught you how to do it, and we are going to do a simple problem and we going to construct this lattice using MATLAB. Suppose we are given the following p4, lattice constant is a is given, 1 atom at Wyckoff position 0.2, 0.3 another Wyckoff position c and another one at a. So, these are the various positions that are there for these atoms. So, how would be go about writing a simple MATLAB program to generate this lattice and what is means. It is very simple it is something, yes.

Student: The terminology abcd, is it universal for all the website there?

Professor: You means this abcd?

Student: Yeah.

Professor: Yeah it will start from a and keep going up, it will start from a at the lowest row and keep going up in general. I do not think there is deviation from that, it is standardized that is precisely the reason so that I do not have to tell you that it is x y, minus x minus y, I will just tell you that there is an atom at 4d, for p4 plain group I will tell you there an atom at 4d you just look up the tables to know what 4d means. What atoms are actually present at position 4d as simple as that. So, what happens is the code that we already looked at is going to be applicable in a straight forward manner, for the fcc crystal structure we defined what is referred to as the bases. We got 4 bases atoms using non primitive lattice vectors to generate the phase centered cubic crystal.

In this case everything remains the same so I am just going to generate one unit cell so I marked n1 0 , n2 0, n3 0 and you have these vectors 1 0 0, 0 1 0 and 0 0 0 because I am creating a plain group, I do not have to have this lattice vector, there is no c lattice vector and then I have a function here which says basis equal to get basis. We will see what that particular function does in just a bit and then the next line is calculating the size of the basis, how many basis atoms are there and then everything is essentially exactly the same as what we did for the fcc crystal structure.

The only thing different is that this line, this is the only line which is different. So, let us see what that line does, this is all that function does. This is another function which is written called function get basis. What am I doing here, I am defining a race with the fractional coordinates of those points given to me. So the first point had fractional coordinate 0.0.2 comma 0.0.3 but I know that it generates 1 minus 0.2, 1 minus 0.3 which basically x bar, y bar form that table. So if you simultaneously if you are able to look at that it will be nice, so the basis d atoms has 1, 2, 3, 4 positions present within that unit cell. 0.2 0.3 which is x comma y minus x minus y 0 which is 1 minus 0.2, 1 minus 0.3 is 0. The next one is minus 1 yx which is 1 minus 0.3, 0.2 0 and the fourth one is y 1 minus 0.2 and 0.

The second one is in position c that is having just half 0 and 0 half which is just written down just like that just half 00 and 0 half 0 and ba is just 000, then I concatenate all these positions bd, bs and ba which is going to be supplied to the main MATLAB program and that will essentially

have the will receive it in the variable basis, so it is a set of all basis for all these points which I am generating in other function and giving it over here. And then when I run this code it will automatically generate the crystal structure.

Since I have given n1, n2, n3 is equal to 0, it will produce one unit cell. So, let us see if that works, so this was the point that was actually given to us 0 comma 0 was given to us. One point at position 4a I think, one point 1 0 comma 0 I gave you, one point at Wyckoff position, another point at Wyckoff position a, Wyckoff position a means what, there is only one point 0 comma 0 that is it.

And then I had these atoms present at the general position, one atom that was present at general position with coordinate 0.2, 0.3, so this is 0.2, 0.3. But on applying this 4 fold rotation, I generated this point, this point and this point. And then I had one more which is present half comma 0. One at Wyckoff position b is what I said, so that is this point and then this point because this is one single unit cell and just generating exactly the number of points that is contained within that unit cell. I don't generate the points that is located at the other end or at x is equal to 1 for example I do not generate the point that is locate at the other end x equal to 1 for example, I do not generate a point at y equal 1 although there must be 1, when it will occur only when I translate it, within this unit cell there are only one, two, three, four, five, six, seven points.

You can find out the total number of points that is going to be present within the unit cell by simply looking at your table, so that should be quite upper and now so there is one atom at 0.2, 0.3 another at c, another at a. So, you go count here so if it as at point d there in multiplicity of 4, therefore there are four atoms in the unit cell and then one at c so there are two more, 4 plus 2 six then there is one at a 0 comma 0, seven. So, you will get seven atoms present per unit cell for this particular 2 dimensional crystal.

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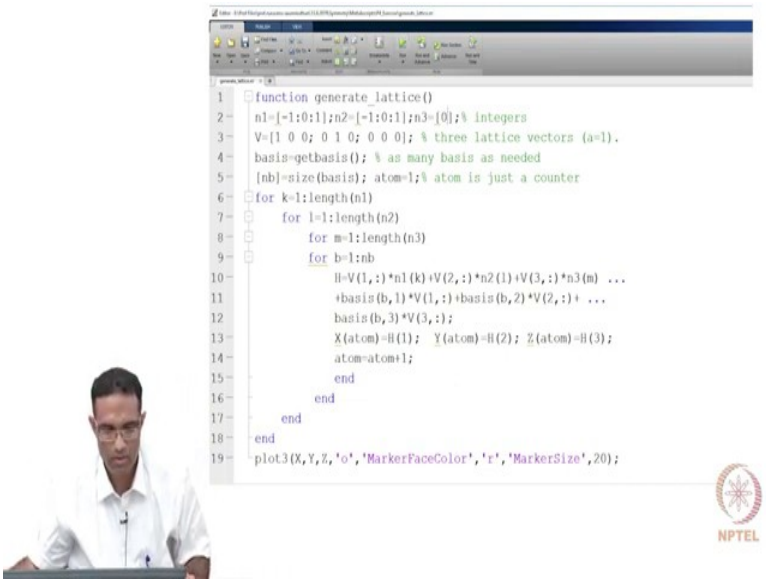

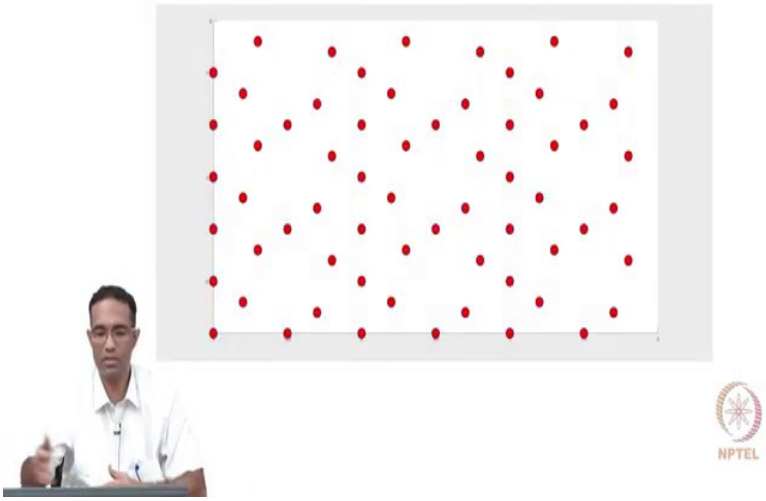

Now this is a very important aspect, if I now changed my MATLAB program to have a couple of different unit cells, say minus 1, 0 to 1, and these are some matter. There is some error here, so that is the entire crystal for some a couple of different lattices, so there is how many lattices are there minus 1 to 1 means there are 2 lattices, there are 2 unit cells in the x2 unit cells in the y direction or three minus 1, 0 and 1. So, you can see the three things here so this one, this is the second one and this is the third one. So the third one is not completing because it is the same atom as this, I should not be putting one atom there, if I put one atom there and repeat this entire

thing two atoms will basically over lap. So, this is all the crystals that is going to be generated when you perform the operation in the manner of that i pointed out.

So, this exercise holds for anything. If I am asking you to create even a 3 dimensional crystal also, the same set of steps will be followed and you can actually create a 3 dimensional crystal and know the positions of all the atoms in your unit cell. It becomes very important, if you are dealing with very simple things, like fcc, bcc and it is very trivia. However if you are dealing with complicated unit cells where each unit cell may contain close to 44 or 50 different atoms, then is just impossible for you to do it without understanding how to do it in a manner that I just demonstrated.

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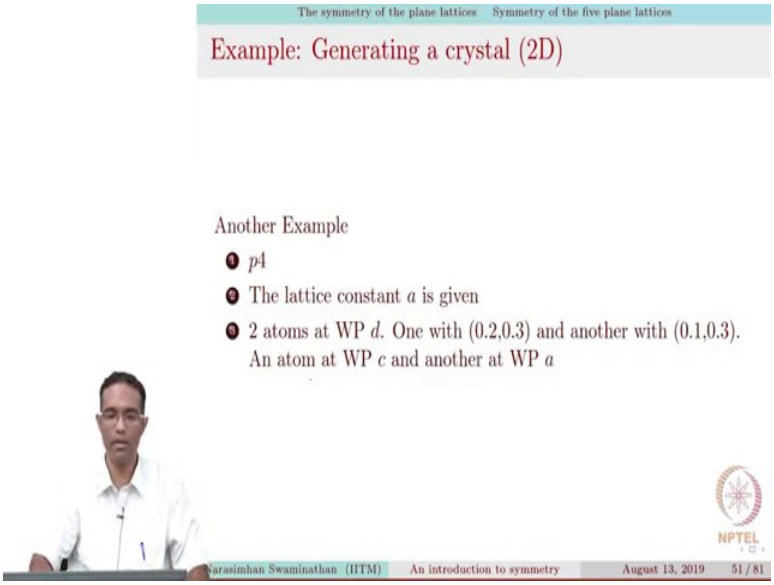

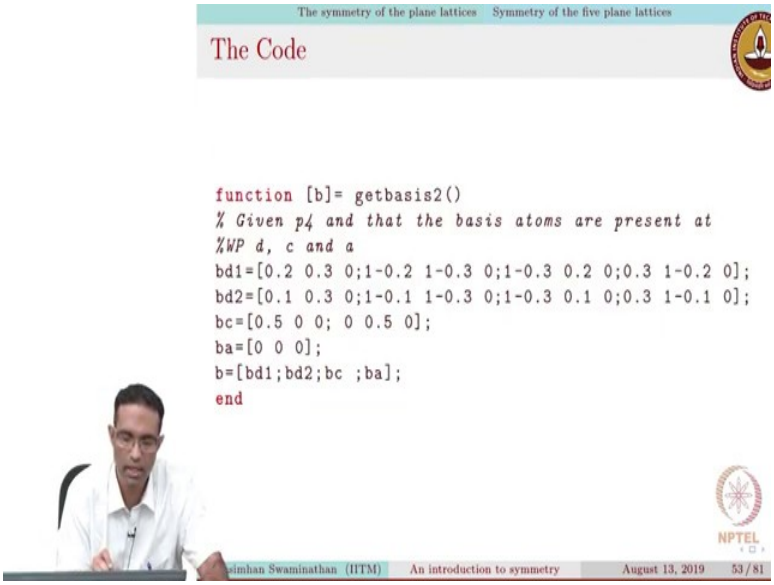

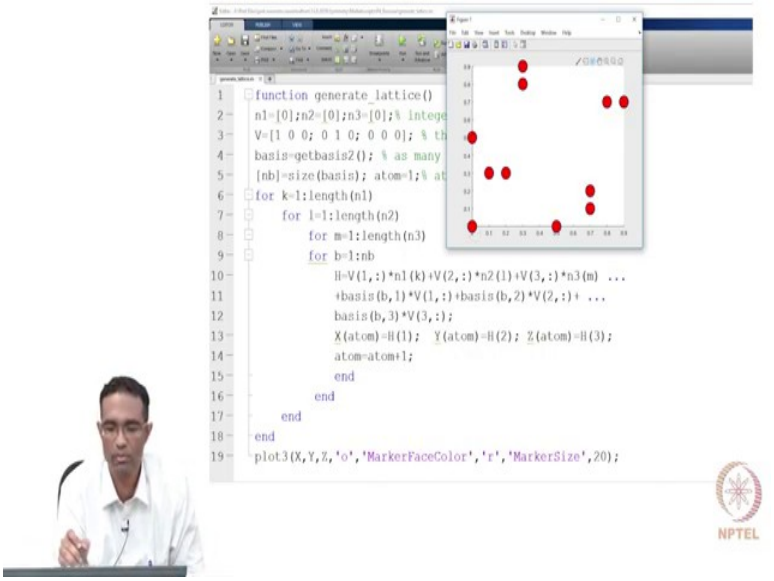

Now we will do one quick exercise, same thing p4, the lattice constant a is given, two atoms at Wyckoff position d now, there are 2 atoms at Wyckoff position d, one with 0.2, 0.3 and another with point 1, 0.3, x comma y. An atom at Wyckoff position c and another atom at Wyckoff position a. So, now if you do the same thing now you have the bd1 and bd2 are the 2 basis atoms at Wyckoff positions d, and the corresponding values have been written down here based on the table which we will study, this is the c, this is the atom at a and I am just conceiting all these atoms and I will generate the crystal.

So, the thing is I just have to do basis 2, which is basically I just have to change the name of the function which returns me the set of the basis atoms and I get a crystal structure a 2D crystal structure and it is a little bit messy, it might not be possible for you to even see that there is actually a 4 fold symmetry in this crystal structure, can be pretty hard. So, let us just take one unit cell and look at it once again, so this is the crystal structure, Convinced? So you have one at 0 comma 0 you have these 2 ones which are at half 0 0 half, which is the position c, and then you should have a 4 into 2 8 atoms being generated from the general position so you do have that one, two, three, four, five, six, seven, eight, nine and ten.

Two atoms being generated from the position and c and from the one that is generated at 0 comma 0. So, this unit cell itself has how many atoms? Eleven atoms. So, you can just now imagine what would happen if you place a complicated molecule, it may be say 20 different atoms at particular positions and apply this space group. It will just the number of atoms per unit cell will be huge.

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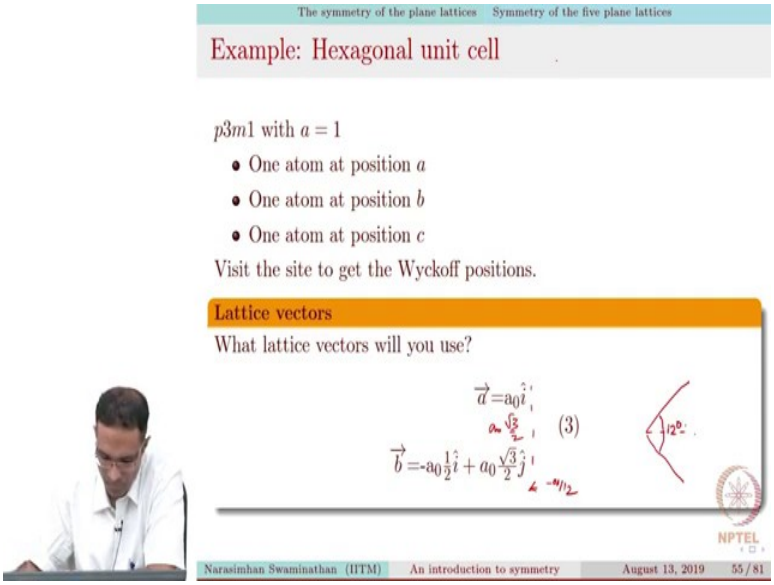
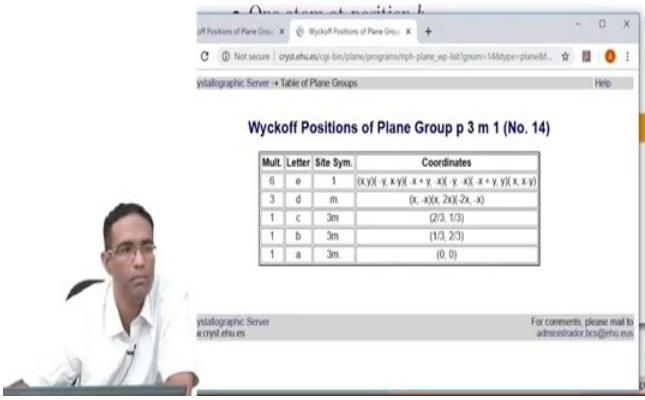


Example: Hexagonal unit cell

$p3m1$ with $a = 1$

- One atom at position a



The symmetry of the plane lattices Symmetry of the five plane lattices

Example: Hexagonal unit cell

$p3m1$ with $a = 1$

- One atom at position a
- One atom at position b
- One atom at position c

Visit the site to get the Wyckoff positions.

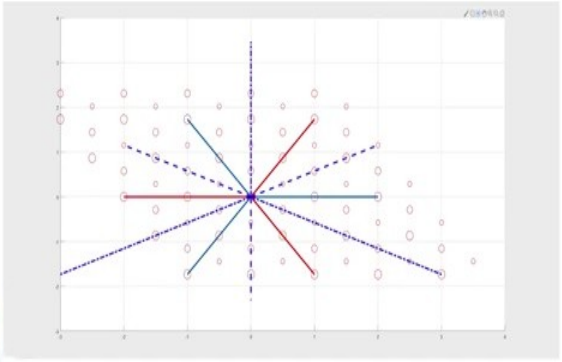
Lattice vectors

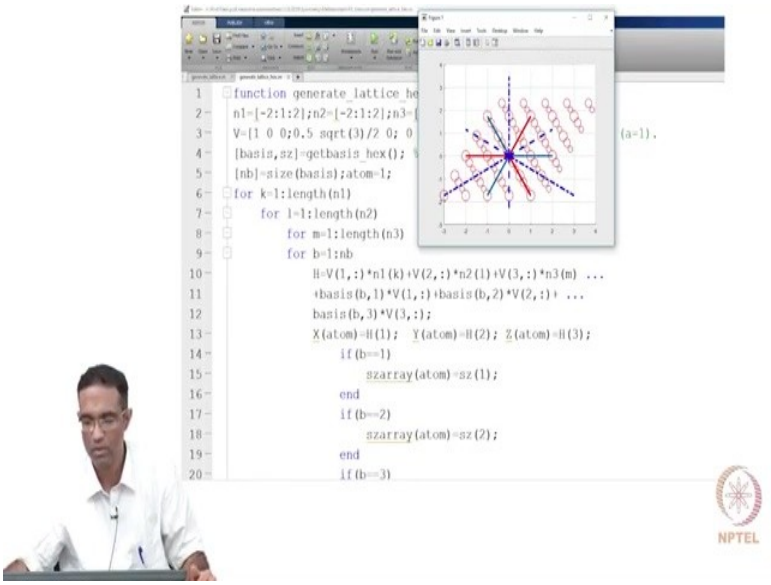
What lattice vectors will you use?

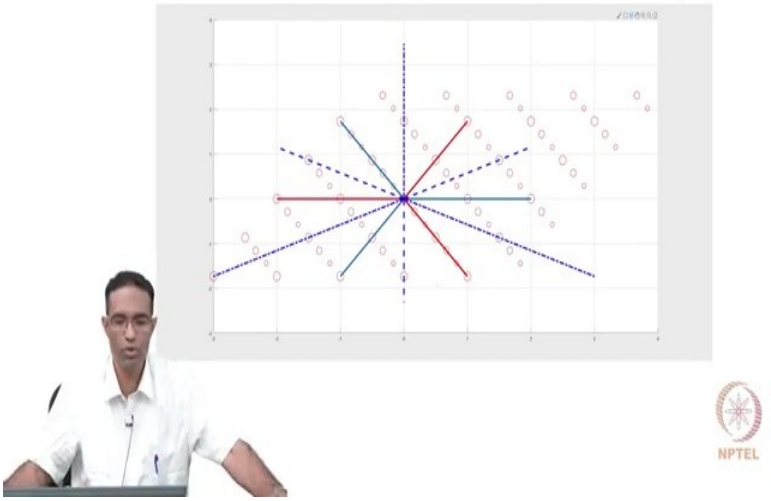
$$\vec{a} = a_0 \hat{i}$$

$$\vec{b} = -a_0 \frac{1}{2} \hat{i} + a_0 \frac{\sqrt{3}}{2} \hat{j}$$

```
function generate_lattice_hex()
n1=[-2:1:2];n2=[-2:1:2];n3=[0:1:1];% integers
V=[0.5 sqrt(3)/2 0;0.5 -sqrt(3)/2 0; 0 0 0]; % three lattice vectors (a=1)
[basis,sz]=getbasis_hex(); % as many basis as needed
[nb]=size(basis);atom=1;
for k=1:length(n1)
    for l=1:length(n2)
        for m=1:length(n3)
        for b=1:nb
            H=V(1,:)*n1(k)+V(2,:)*n2(l)+V(3,:)*n3(m) ...
            +basis(b,1)*V(1,:)+basis(b,2)*V(2,:)+ ...
            basis(b,3)*V(3,:);
            X(atom)=H(1);  Y(atom)=H(2); Z(atom)=H(3);
                if(b==1)
                    szarray(atom)=sz(1);
                end
                if(b==2)
                    szarray(atom)=sz(2);
                end
                if(b==3)
```







So, now let us look at slightly different unit cells, other unit cells are pretty straight forward, you have the rectangular unit cell, so all you going to do is change the value of a and the b, they are not going to be equal anymore and then you are going to have the third kind of unit cell that you will have is a hexagonal unit cell but I want to talk about the particular hexagonal unit cell which has the 3 fold symmetry only associated with it. So, the given problem is the 2 dimensional crystal is in the space group p3 m1, with a equal to 1, one atom is at position a, one atom at position b and one atom at position c, this is all that is given to us. So how would we go about generating the crystal structure, so the first as usual corresponding website right here, p3 m1 and it tells you, again it starts from a to e, it tells you that the general points x comma y generates 6

additional atoms within the unit cell, an atom at b generates 1 and another atom at c generates 1, 2 by 3, 1 by 3, 1 by 3, 2 by 3.

So, the multiplicity is given here 6 different atoms that would be generated by performing all operations corresponding to this plain group on this general atom is given here, then you have points with multiplicity 1, 1 by 3 2 by 3 and 2 by 3 1 by 3, so would we go about generating the crystal structure, 2 dimensional crystal structure. Firstly it is important for us to choose a unit cell, in the case of the square measure it was very obvious what we needed to choose as a unit cell. Unit cell means what, the corresponding lattice vectors, so in hexagonal case as soon as you see p3 or p6, it should strike to you that it has got to be a hexagonal lattice that applies even for space lattices, so what we can do is we can chose this to be over one of the lattice vectors, the other one is chosen to be this. This is equal to minus a not by 2 and this one is root 3 by 2 into a naught such that the inclined angle between these two vectors is 120 degree.

It does not work if you chose this as b, only this has to be chosen as b. That works for both, hexagonal lattices with 3 fold rotational symmetry and lattices with 6 fold rotation symmetry. So we will choose a as this, b as this, and construct over lattice. So let us take a look at our MATLAB court for doing this, so this is my MATLAB court for doing that, so I am going to generate 2 or minus 2, 2 plus 1 3 plus 2 5 unit cells in the x, 5 unit cells in the y direction. So, I am going to change this lattice vectors to be what I just wrote down on the slide, so I am going to say this is 1 0 0, and the other one was minus 0.5, square root of 3 by 2 0, what is that?

Student: The first one is 1 0 0 .

Professor: Sorry, thank you this is what it generates. So let me just generate it again, the lines that have been drawn are all the ones which have 120 degree include angle between them. The dash lines, the dotted lines, and the thick red lines, the thick wherever the other color lines and the dotted dash lines, they are all having an incline angle of 120 degree between them. So, the environment along those lines should all be the same because this 2 dimensional crystal has the 3 fold symmetry in it, so let us take a look at this line, what color is that by the way?

Student: cyan.

Professor: cyan , so, you have 2 atoms here, 2 atoms here, 2 atoms here looks exactly the same, similarly you take the red one, you have 2 big atoms here, 2 big atoms here and 2 big atoms here. Now you look at the dash lines, so you have one medium size atom, small atom and the big atom, so it is perfectly having this 3 fold rotation in this picture, like what it should have. If you had not chosen the lattice vectors correctly and for some reasons incorrectly chosen the one I just wrote it down which is basically 1 0 0 0.5, square root of 3 by 2 0 which is the one with 60 degree included angle, which is the mistake that you can make thinking that you know it just needs to be 60 degrees. Now still it must if it has the 3 fold rotation it must look like it has the 3 fold rotation, does it has the 3 fold rotation? No.

You see it does not have, so choosing this unit cell is extremely important, the red ones which have 120 degree between each other, this one has line of medium atoms, small atoms and the big atoms and repeating itself. Whereas these two are different from this. So if you rotate it by 120 degrees they do not really coincide, they do not have 3 fold rotation. so, you have to chose unit cells carefully. We can choose any set of vectors which have included angle 120 degrees between them. Another choice would be 0.5 square root of 3 by 2, 0.5 minus square root of 3 by 2 which is this, what am I choosing here so I would write neatly, this is what I am choosing. Now or the things having the 3 fold symmetry, yes. so this is an important aspect to remember when you are constructing hexagonal lattices. What is the symmetry that you are dealing with, there are 3 fold symmetry or 6 fold symmetry.

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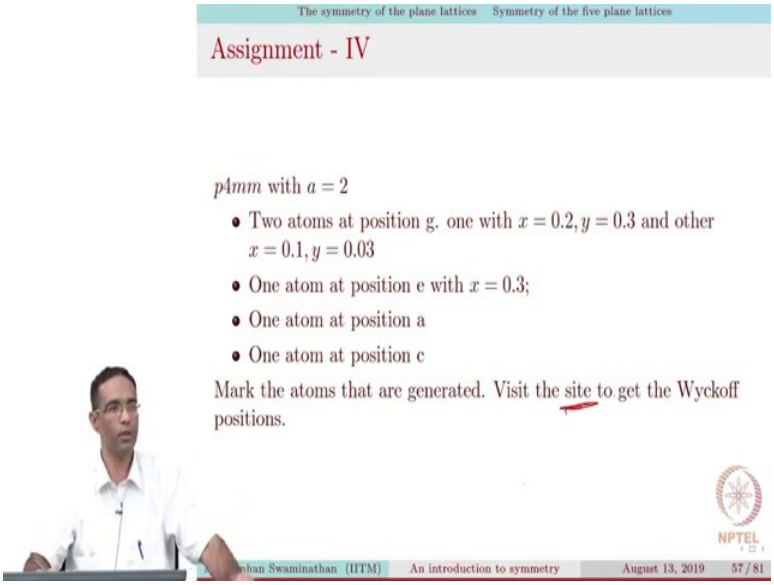

So, the next I have given you a quick assignment here it should be very easy to do, all you have to do is click on this link right here and it will take you to the table which has the p4 m1 all the Wyckoff position associated with the p4 and m. And you are expected to use this MATLAB to actually generate the 2 dimensional crystal. Should be very simple.