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Phase field modeling; the materials science, mathematics and computational aspects

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Module No.12
Lecture No.50
Crystal: symmetry
Elements II

Welcome we are discussing symmetry groups group is a set of elements with an operation defined for adding or multiplying the group elements and under the operation these elements satisfy certain properties first is called closure so if you take any two elements and if you do this addition or multiplication operator operation you end up with an element which is also in the same set the second one is known as associatively it says that if you have three elements ABC belonging to a group whether you multiply BC first and then left multiply A to it or you multiply AB and left multiply that to see does not matter.

So this is known as associatively and then there is a unit element which if you multiply with all the other group elements you end up with the same element and there is also an inverse element for every element there is an inverse element which if you multiply with the element you will get the unit element so if any set of elements under some given operations multiplication or addition it is called group addition or group multiplication obeys these four properties then we call that as a group.

Now we also defined what is known as asymmetry group what is the symmetry group so we considered an equilateral triangle.

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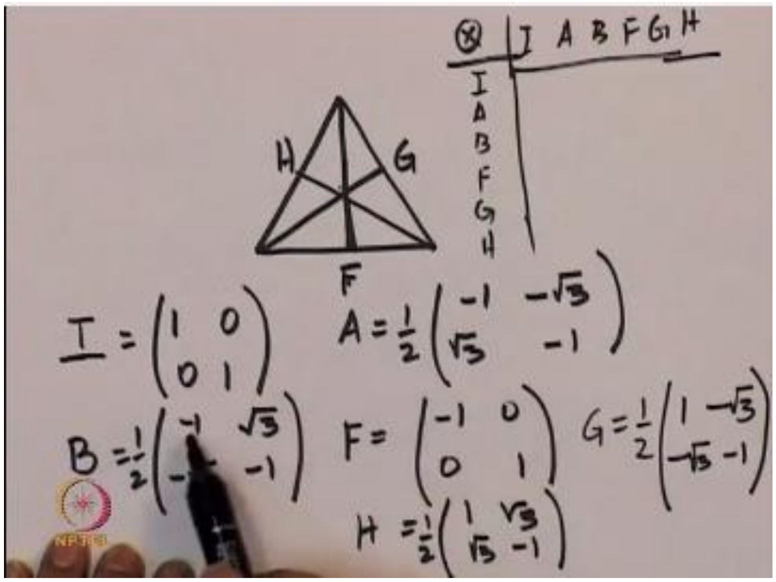

And we defined symmetry operations and those operations are about the CFG for example you can rotate120^0 so 120 240 and 360 is basically equivalent to 0^0 rotation so those are three and then we also had reflection operation so we defined some three lines which pass through CFG and which are perpendicular bisectors of the opposite side about which you reflect for example so we define this I think as F G and H so the operations the three rotation operations and the three reflection operations and under the combination for example you do one rotation you follow it by another rotation or you do one rotation and then you do a reflection right.

So that is the combination is a group so that we saw last time and there is another way to represent the same group and that is as follows so the elements of the group can also be represented by matrices of course first is the I operator which is the unit element which is nothing but 10 0 1 the second one is a which is 120^0 rotation which is given by and the third one is 240^0 rotation and this is given by and then the reflection operation F is defined by okay, and the because the reflection operation F you know takes the X point 2 minus X but it leaves y unchanged I mean that is that is what this operator is.

And the other two reflections G and H are similarly defined g is and H operator is defined like this now all these six elements so you can make a group table like we did last time so you can call I A B F G H and I A B F G H you will see that all the elements are I A B F G H only and I happens to be the unit element and for every element you can find out the inverse element and these operations which are basically if you consider I A G I A B of GH as these matrices the multiplication operation the group multiplication operation is nothing but the matrix multiplication.

So under the matrix multiplication you will get the properties and the notice that because these are matrix multiplication they are generally not commutative A x B does not necessarily mean B x A if in a group it happens to be so such a group is called a billion and if it is not it is non a billion so this is the symmetry so these are the symmetry elements of equilateral triangle and it forms a group so this is known as asymmetry group so this is the symmetry group for an equilateral triangle.

With this idea in mind we now want to define what is known as the point group symmetry of a crystal because remember we are doing all this exercise to understand the Nyman's principle which says that the physical property of a given crystal should include the point group symmetry of that crystal okay so we need to understand what is the point group symmetry and then we also need to understand how we define the symmetry of any given property to understand a point group symmetry let us start with what is the what is known as a lattice so what is the lattice.

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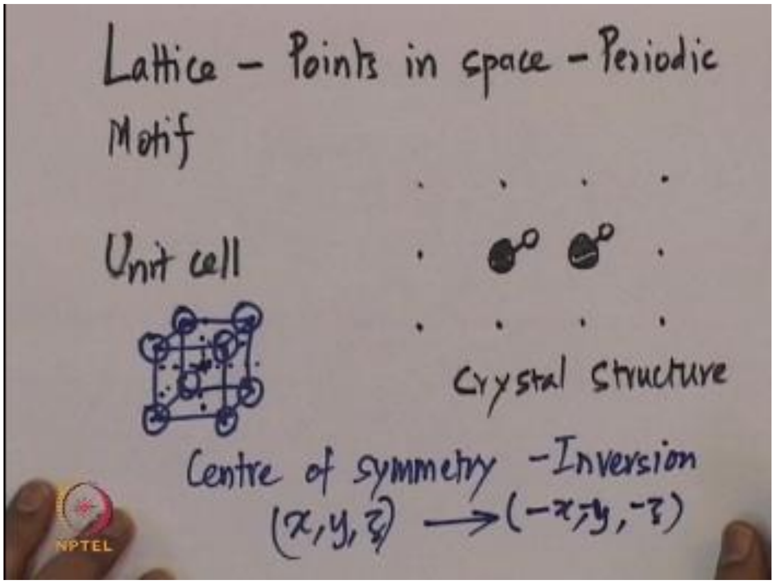

Lattice okay is basically points in space which are periodic okay so the periodic array of points in space is known as lattice and if with every lattice you associate certain atoms or molecules and the atoms or molecules that you associate is known as a motive okay, so if you associate for example I might have this as my lattice okay and this continues both the directions both x and y directions this is infinite it continues and if I associate for example with every point a set of items right suppose v4 and if I repeat this so everywhere I do this.

It though this will be called the motive and the lattice surplus motive actually makes the crystal structure so this crystal structure then can be explained in terms of what is known as a unit cell right so there are many different unit cells for example the simple cubic unit cell is the one which will be a box like this cube and which has atoms probably at every point right so note that this could be an atom this could be a molecule so anything that you can put but now for simplicity sake I am just taking atoms and I am putting at the lattice position so this is the unit cell now like we did in the case of equilateral triangle you can take a shape like this undefined certain symmetry operations.

Those basically form these symmetry elements what are the symmetry elements there are many but we are going to define what is known as the fine group so there are certain symmetry elements that we will discuss so what are those symmetry elements one is known as centre of symmetry or it is also known as inversion this what we do for example you take the center of this unit cell and suppose you had the X Y Z axis you invert all of them x goes to -X Y goes to –Y Z goes to -X so X, Y, Z, goes to - X -Y – Z.

Okay so this is a symmetry operation ok this is known as either immersion or center of symmetry so this is one symmetry operation so it is a symmetry element, the second symmetry operation that we want to define is known as a mirror plane okay so what is a mirror plane.

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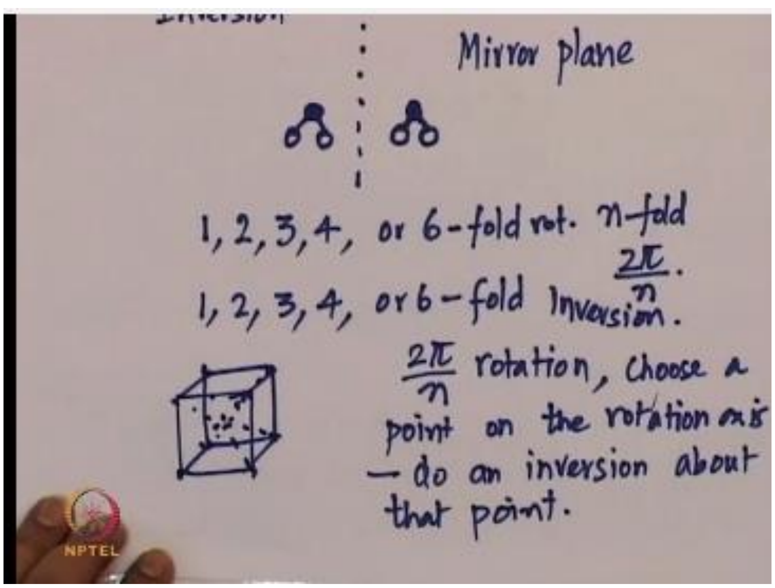

So suppose you have a set of elements like this right something like this right suppose if I take a plane about which I mirror this right so this is a mirror plane and so this is a symmetry operation so mirror plane is a symmetry operation so center of inversion is one mirror place is mirror plane is another then you can have rotation and the rotation could be one fold two fold three fold fourfold or 6 fold what is this a fold mean if it is n fold you rotate by $2\pi/n$ that is what tenfold means.

So two-fold means you rotate $2\pi/2$ so that is π that is 180^0 rotation threefold means $2\pi/3$ and so 2π is 360 x 3 is 120 so in the case of equilateral triangle what we had is basically a threefold fourfold means 90^0 rotation and the six fold means 60^0 rotation one fold basically means 2π rotation which means you do not rotate it at all 360^0 there is no rotation then there is what is known as inversion and those are one fold twofold threefold fourfold or six fold so this is rotation and this is inversion.

In this case what we do is that we do a rotation right off of whatever $2\pi/n$ rotation and then we choose a point on the rotation axis choose a point on the rotation axis and do an inversion about that point now the inversion so let me write it here inversion mirror plane and the n-fold rotation and n fold inversion these are symmetry elements they form a group so that is known as a symmetry group and this is known as a point group symmetry and the name comes from the fact that when you combine these operations all these operations can be thought of as being done about a point right.

In other words we are looking at the symmetry operations which do not involve any translation so we are lattice is you know repeating the same sort of point structure in space indefinitely in all three dimensions right so that is how you get a lattice so that is a mathematical concept and with each lattice point if you associate a motive then you get what is known as a crystal structure and the crystal structure can be described in terms of unit cells now when we are thinking about the point group symmetry.

We are thinking about this unit cell and sort of what are the macroscopic symmetry operations that you can do on them so those are the symmetry elements and I consider only those symmetry elements which can be thought of to be carried out about a point for example you can have a point you can have an axis through the point about which you will do rotation you can have a plane which consists of that point about which you will do reflection and about the point you will do in version so everything is with respect to a specific point which means the translation is not something that we worry about so the group that you form with these symmetry elements for the unit cell is known as a point group symmetry.

So we have defined one part of the Nyman's theorem which says that the symmetry of any given property of a crystal should include its point group symmetry so now we know what is a point group symmetry what is the point group symmetry these are symmetry operations which are inversion mirror plane n fold rotation and n fold inversion and they form a group so that is the point group symmetry for example if you think of the simple cubic unit cell that I described a while back.

So the one of the important point of symmetries of this cube is that it has a threefold rotation about 4 axis and those 4 axis or the diagonal ones you know from here to here from here to here and from here to here and from here to here so there are four of them and you have threefold axis about these four I is as I mean that is one of the important symmetries that this cube has for example and in the case of FCC it is easier to see so that will be basically the 1 1 1 plane so these are the kind of operation.

So these are the kind of symmetries that exists with respect to the macroscopic symmetry operations on a unit cell and that forms a group and that is known as the point group symmetry so we know what symmetry is symmetry is any operation that leaves the object unchanged it could be a mathematical object it would be a physical or could be a geometrical object and the operation could be a mathematical operation or a geometric operation and under that operation if the if the object remains unchanged then we call that as symmetry.

And the element the symmetry can be described for example we decided to describe the symmetry of the triangular equilateral triangle using rotation matrices or and reflection matrices so you can use matrices to represent so they basically become these symmetry elements because these operations form a group when they are combined with each other for example you do an inversion and then you do a rotation you do a rotation and then you do a mirror so these operations combined together so that combination.

So if you think of these group elements as matrices these are just matrix multiplication so way of combining these matrices then they form a group or so that is the point group symmetry because we are only considering those symmetry elements which can be thought of to be carried out about a point with respect to the unit cell okay, so we consider some point in the unit cell about which we do all these operations so it is known as point group symmetry.

And so we now have an idea of what it means to say that the point group of symmetry okay so now this the property should have a symmetry which includes the point group symmetry so what does it mean to say that the property has some symmetric okay so that is what we will discuss in the next part of this lecture. Thank you.

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