3D Space Groups I: Introduction
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Lecture 22 a

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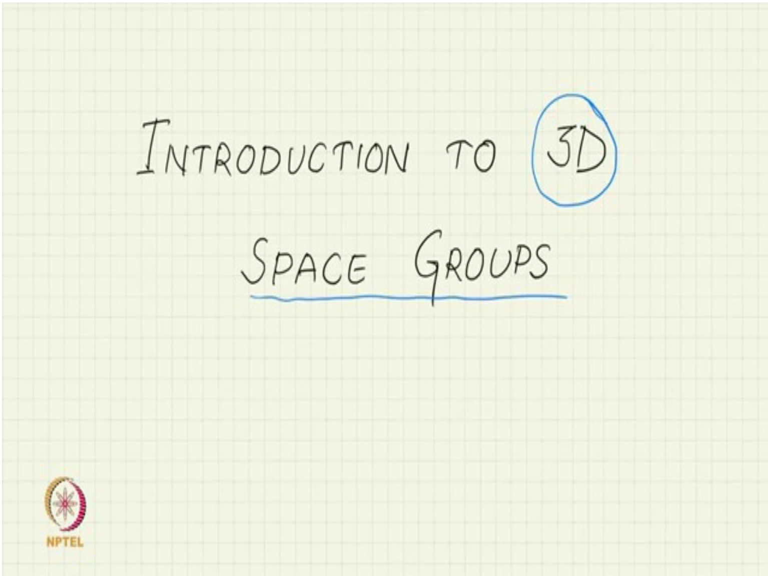

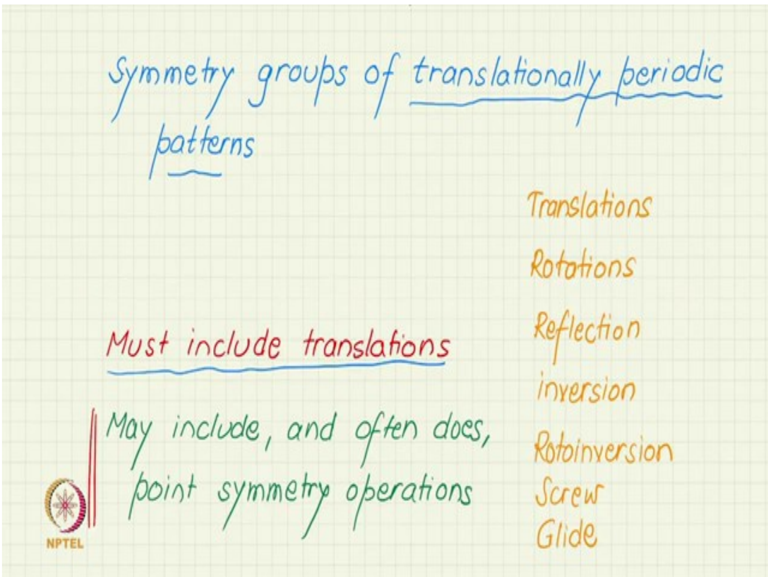

The time has now come to venture into 3 dimensions. So, we will now discuss 3 dimensional space groups. We have looked at in detail the 3 dimensional Point groups, but now we will see how we will develop the space groups using those Point groups. So, space group is symmetry group of translationally periodic patterns. So, since translational periodicity is required it must include translations. But beyond translations it may also include and often does different point symmetry operations. So, if you make a list of all possible operations in a space group. So, you will have translations which are required. When you can have rotations and often you will have rotations, then you can have reflection, inversion, Rotoinversion, screw and glide.

So, a combination of all these operations these operations combine in a certain way and in fact as we will see there are 230 different ways of combining them we cannot really go into the details of derivation of these 230 space group but through examples of some of them, we will try to understand how these operations combine and give you some specific space groups.

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So, space group, although we are starting 3 dimensional space group in this video, it is not that we are meeting a space group for the first time in the series of lectures. We in fact, have met a space group with different names. So, if the dimensionality of a space is 2, so a 2 dimensional space but if translational periodicity is only in One Direction. One, then we have a space Group which we called in this special case a freeze group. So, freeze groups are nothing but space groups of 2 dimensional patterns with one dimensional periodicity, and in this case we have seen that in some previous videos that there are 7 freeze groups in total. So, we can say that there are 7 space groups of this type.

Then the second example which we have considered is 2 dimensional space with 2 dimensional periodicity, this is what we call plane groups, and here we found that there are 17 different types of plane groups. So, plane groups are also space groups but space groups of 2 dimensional patterns with 2 dimensional translational periodicity.

But finally, now the time has come to discuss 3 dimensional space with 3 dimensional periodicity, this is what we usually call space groups or we can call them 3 dimensional space group, but if we do not qualify, use any adjective simply say space groups it means usually the 3 dimensional space group with 3 translational periodicity. And in this case, the number blows up to 230. So, there are many possible combinations of those symmetry operations which I just showed you.

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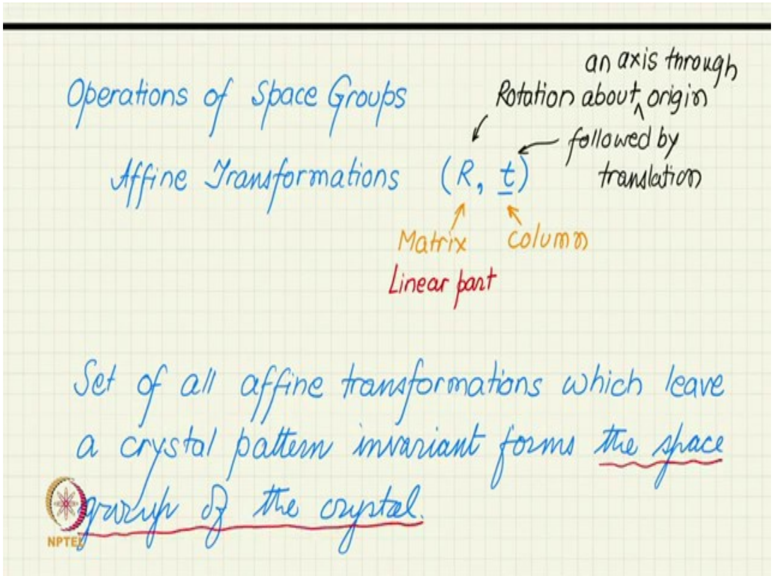

So, symmetry operations we have seen also in the case of 2 dimensions, that symmetry operations are represented by affine transformation and affine transformation is a combination of a rotation followed by a translation. And in space group rotations can be about many different axes or axes located in different positions in space they can be in different orientations and they need not be intersecting, they can be in different parts of a space. So, but here when we write the affine transformation, we write rotation always about the origins. So, the axis should be passing through the origin.

So, exact way of writing with to be rotation about an axis through origin. So, sometimes the rotation, since the rotation part is represented by a matrix this is also sometimes called a matrix part and the translation is represented by a column Vector, this is called column part. So, a fine transformation is also a combination of Matrix and column as their representation. And Matrix also represents a linear transformation, sometimes the Matrix part is also called a linear part of the transformation.

Now, the space group is nothing but all possible such combinations which will leave the crystal pattern in variant. So, atoms will move, but each atom will move to some other equivalent position such that the overall appearance of the crystal does not change. So, set of all affine transformations which leave a crystal pattern in variant forms the group and this is what is called the space group of the Crystal.

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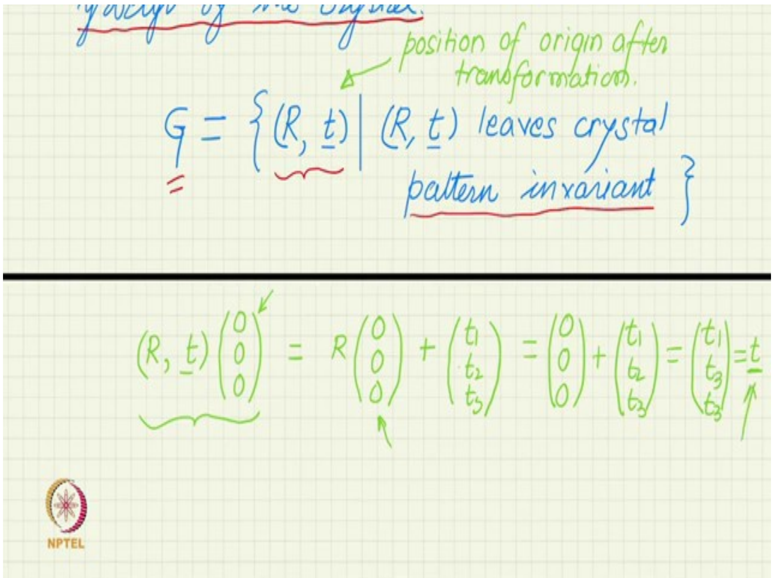

So, we can say that space group of the Crystal G each set of all affine transformation R t with the property that R t leaves the crystal pattern in variant then only it is a symmetry operation.

Now, we can have various kinds of these fine transformation. So, a special kind of a fine transformation in which the rotation part is an identity, then there is no rotation really. So, identity followed by translation is simply a translation, and that translation, if it leaves the Crystal and pattern invariant has to be lattice translation. So, in the space group, if we have any affine transformation as having the linear part as Identity or the Matrix part as identity that means it represents a pure lattice translation.

You can have pure rotation leaving the origin fixed written as R o. Note that, this translation part, the translation part of R t, translation part of R t can also be interpreted as the position of origin after transformation. So, in any affine transformation the column part or the translation part is the translation of the origin due to that affine transformation, this is not difficult to see, we can we can try to say this.

So, to prove this fact all you have to do is to apply your R t to the vector the 0 Vector which is representing the origin. So, then or you can write it as write it as a column vector the origin is represented by 0 0 0. So, that means by the definition of a fine transformation you will have R o o o plus the translation Vector t which let me write as again as a column vector t1 t2 t3. So, t1 t2 t3 is the representation of t in the relevant coordinate system.

Now, any Matrix when it multiplies a 0 column Vector will always give you only 0 vector 0 plus t1 t2 t3, you are left with t1 t2 t3 which is what is the representation of t. So, you can see that if you try to transform the origin by the affine transformation it goes to t, which is the column part of the affine transformation. So, this is what we wanted to show here.

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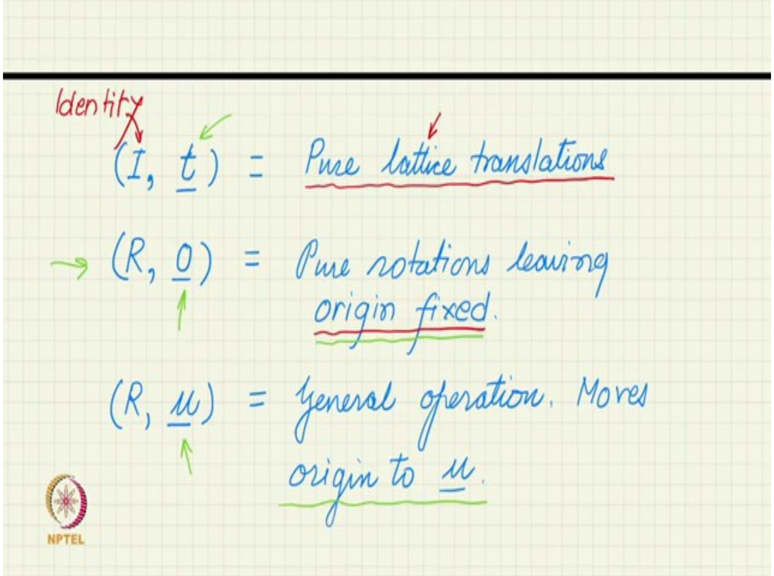

So, if you take this, if there is 0 Vector at the column part, then that means it is a pure rotation and origin is not moved origin is fixed your origin is not translated, then only the column part will be a 0 vector. Then you can have a more General operation where the origin moves to the vector u we have already seen this, I am writing it u to distinguish it from t. So, t, I am trying to accept as lattice translation and u as a general translation.

So, in a space group, you can have affine transformation in which the translation part is not a lattice translation, that happens for 2 operations which we have met and that is this screw and glide. Both of these operations involve translation but they involve fractional translations and not a complete lattice translation. So, if the affine transformation is representing the screw operation or a Glide operation, then this u will not be a lattice translation, u need not bear lattice translation, for example, in case of screw or glide.

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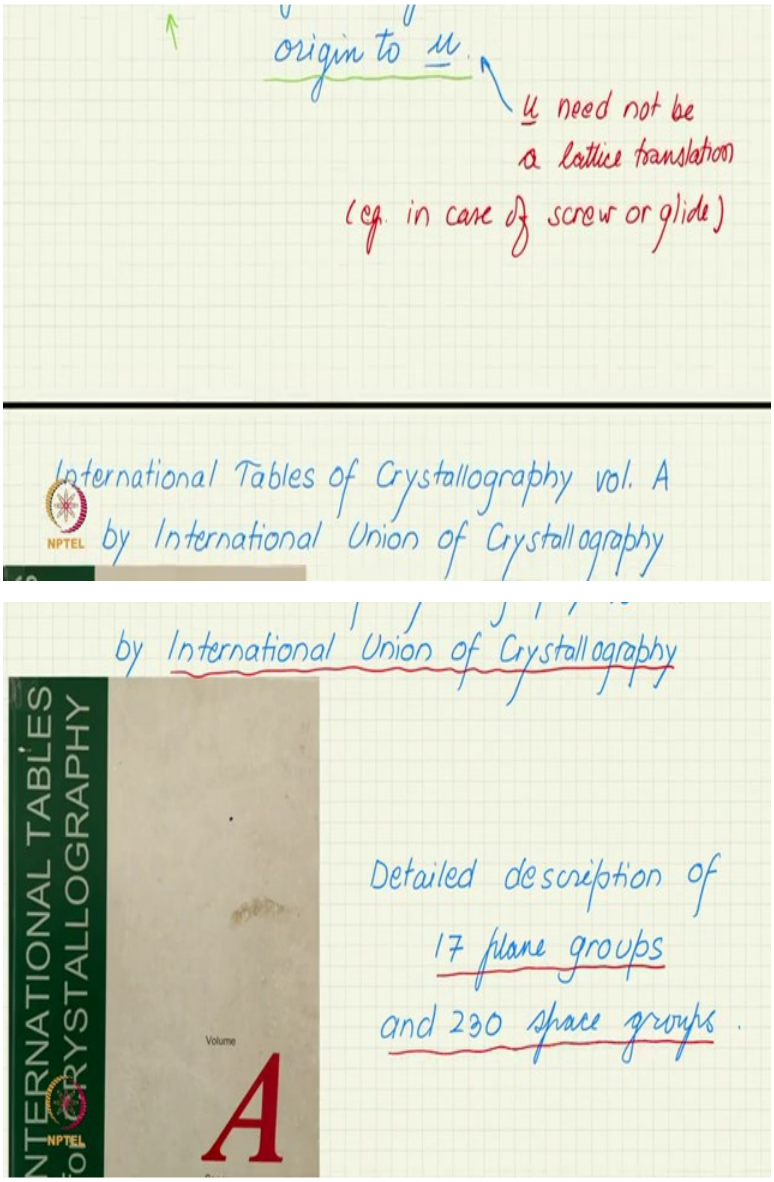

Now, all the details about the 230 space Group, which you want to look for all these details are available in one solid book called international tables of crystallography, this is published by International Union of crystallography, there is an international Union, and they published this book international tables of crystallography, it has complete detailed description of all the 17 plane groups which we have discussed previously and the 230 space groups which we will now be discussing.

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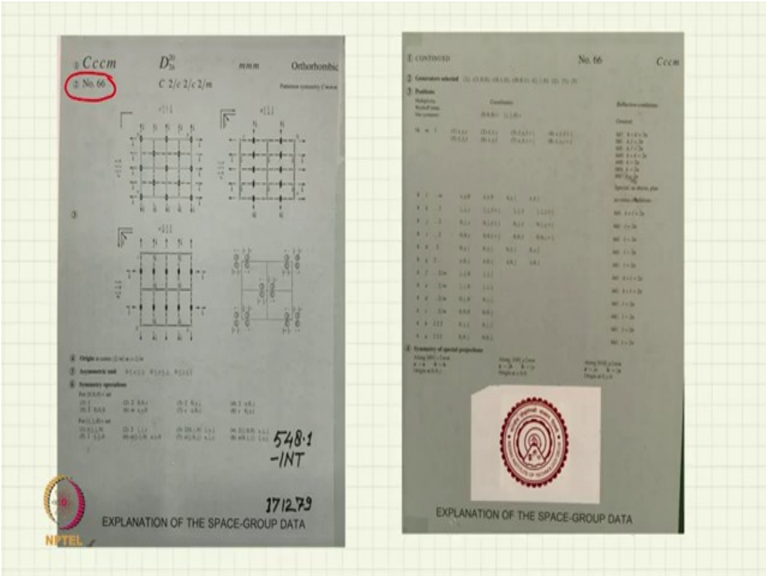

So, let us open this book and look at some page. So, in fact the book itself has guide to read the tables and these pages are taken from that guide, they are in the inside cover of that book. So, here, a particular space group, in this case, space group number 66. So, all 230 space groups are numbered from 1 to 230 and this particular example shows you the space group number 66. So, all detailed information about the space group is there in these 2 pages devoted to this particular space group. We will discuss these details in later videos.

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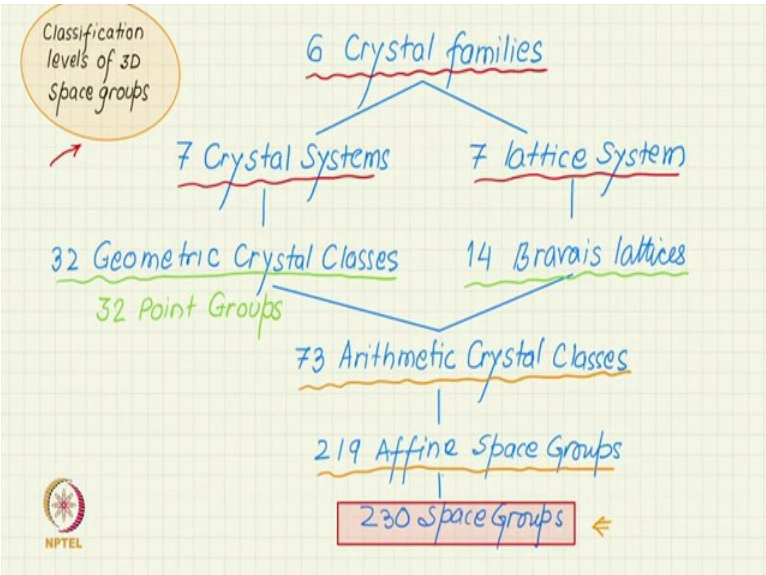

Let me just introduce you in again in this book you will find a classification scheme of a space group. So, different classification level. So, one of the most coarsest classification, coarsest means one leading to least number of categories least number of divisions is the so-called Crystal family. So, all space group can be divided into 6 Crystal families. A finer division from 6 Crystal families age of 7 Crystal systems or 7 lattice systems. One has to be careful although the number is 7 in both cases, the 7 Crystal systems are not identical with 7 lattice system we have a video devoted to this distinction and will come later. So, I will not spend time at this moment.

Then you have 32 geometric Crystal classes, these are nothing but 32-point groups which we have discussed. So, each space group, each of the 230 space groups will belong to one of the 32-point groups. In the lattice system side, you can have 14 Bravais lattices again each of the 230-space group will belong to one of the 14 Bravais lattices.

Lower down in this classification more finer classification is into 73 arithmetic Crystal classes. Again, we will take up this concept in a separate video 23 arithmetic classes, finally, you go to 219 affine space groups and you end up with 230 space groups as the finest classification. So, all these are different classifications, one way of looking at all these terminologies or all these phrases at that they are classification of 3 dimensional space groups using different features or different characteristics. How do we do that? We will look at in the coming videos. Thank you very much.