Crystals, Symmetry and Tensors
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Lecture 9b
Matrix Representation of Symmetry Operation-II

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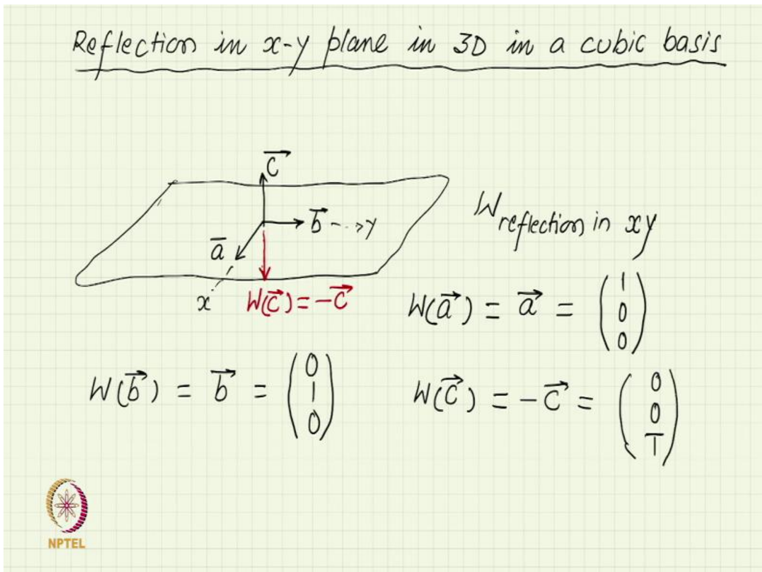
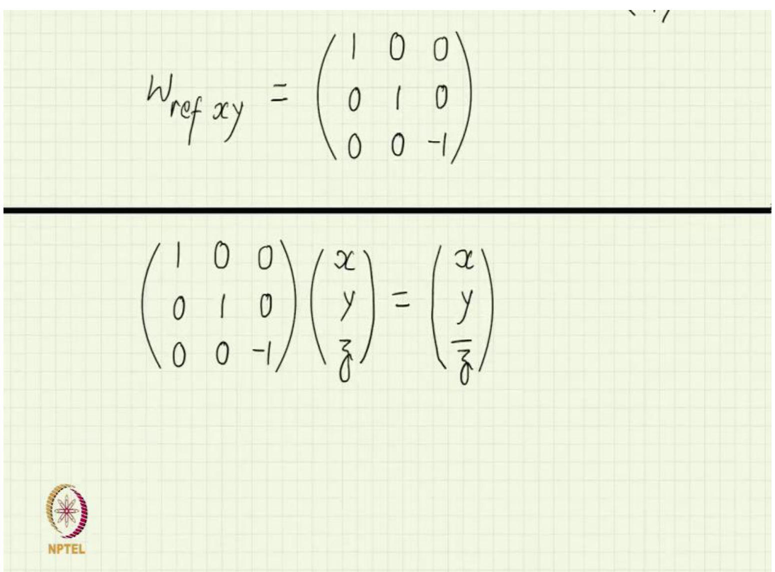
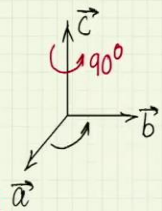




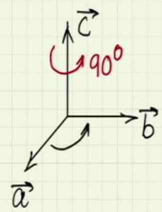
$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} x \\ y \\ \bar{z} \end{pmatrix}$$

Rotation by 90° CCW about z-axis in cubic system



$$\begin{pmatrix} 0 & \bar{1} & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Rotation by 90° CCW about z-axis in cubic system



$$\begin{pmatrix} 0 & \bar{1} & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Det $= +1$ No change in Handedness

Type I or Proper operation

$$W(\vec{b}) = \vec{b} = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \qquad W(\vec{c}) = -\vec{c} = \begin{pmatrix} 0 \\ 0 \\ \bar{1} \end{pmatrix}$$

$$W_{ref\ xy} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

Det $= -1$ Change of Handedness

Improper Operation or Type II Operation

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} x \\ y \\ \bar{z} \end{pmatrix}$$

Rotation by 90° CCW about z-axis in cubic system

So, let us generalize to reflection in 3D. But we take a cubic basis for simplicity. But it does not have to be cubic. It is total general, it is independent of the coordinate basis and it is independent of the kind of symmetry operation you are having. So, let us do this, this is the x axis, this is the y axis, so, I want to write the reflection matrix W representing reflection in xy plane what we have to do we have to find W a where will a reflect if it is reflected in the xy plane louder.

Student: Not change sir.

Professor: Cannot change this is what is called in invariant vector some operations leave some of the directions or some of the vectors unchanged. So, reflection in the xy plane will leave a unchanged. So, Wa is a, a in x the abc coordinate system is 1 0 0, Wb same remains b, b in x original coordinate system is o 1 o, Wc will do something interesting what will it do? Because, if you are reflecting in the xy plane instead of pointing it pointing up, it will point down and it will be a vector of the same length, so Wc is nothing but minus c and minus c in our coordinate system is 0 0 minus 1.

So, reflection W representing the reflection in xy plane will become transformed a which is 1 0 0, transformed b which is 0 1 0 and transformed c which is 0 0 minus 1. So, this completely represents the reflection of any general vector and you can see if you multiply it with any general vector x y z what will it give you? This matrix.

Student: x y z bar.

Professor: x y z bar. Now, if you are reflecting any vector in the xy plane, this is what you expected it, is not it? It should not change its x coordinate, it should not change its y coordinate and it should make the z coordinate negative. Now, this also shows an interesting so, let us write rotation also, which is also simple. Now you got the idea I have cubic a b and c. So, they are equal in length angle is 90 degree and I am rotating by 90 degree about c about z axis and of course, I am forgetting to write CCW. So, counterclockwise, so, what is the matrix?

Student: c will remain same.

Professor: c will remain same you are telling about the last column, so 0 0 1.

Student: First will be 0 1 0.

Professor: Because the x axis goes into b 0 1 0.

Student: Minus 1 0 0.

Professor: Minus 1 0 0. Everyone is comfortable with them. Now, let us establish some property a1 property of the determinant of these matrixes, what is the determinant of this rotation matrix?

Student: 1

Professor: 1, what is the determinant here of the reflection?

Student: Minus 1

Professor: Minus 1, this difference in determinant is actually having physical origin in terms of?

Student: Handedness.

Professor: Handedness. What does reflection do to handedness?

Student: Handedness change.

Professor: Handedness change. So, reflection will always reflect a right handed glove into a left handed glove or right handed object into a left handed object. So, if a random matrix is thrown at you without telling that what it is. So, if you determine its the just the sign of determinant, you can at least tell whether it changes handedness or not. If the negative determinant is negative, there is a change in handedness if determinant is positive, no change in handedness. Crystallographers use a jargon here.

So, let us get familiar with that. Operations which change handedness are called somehow I do not know why they should be called improper but they are called improper there is nothing improper about them. They are called improper operations or sometimes type II operation, this is just the definition that an operation which chain handedness that is whose determinant will be minus 1 is an improper operation or a Type II operation. The one which do not change handedness is a Type I or proper operation.

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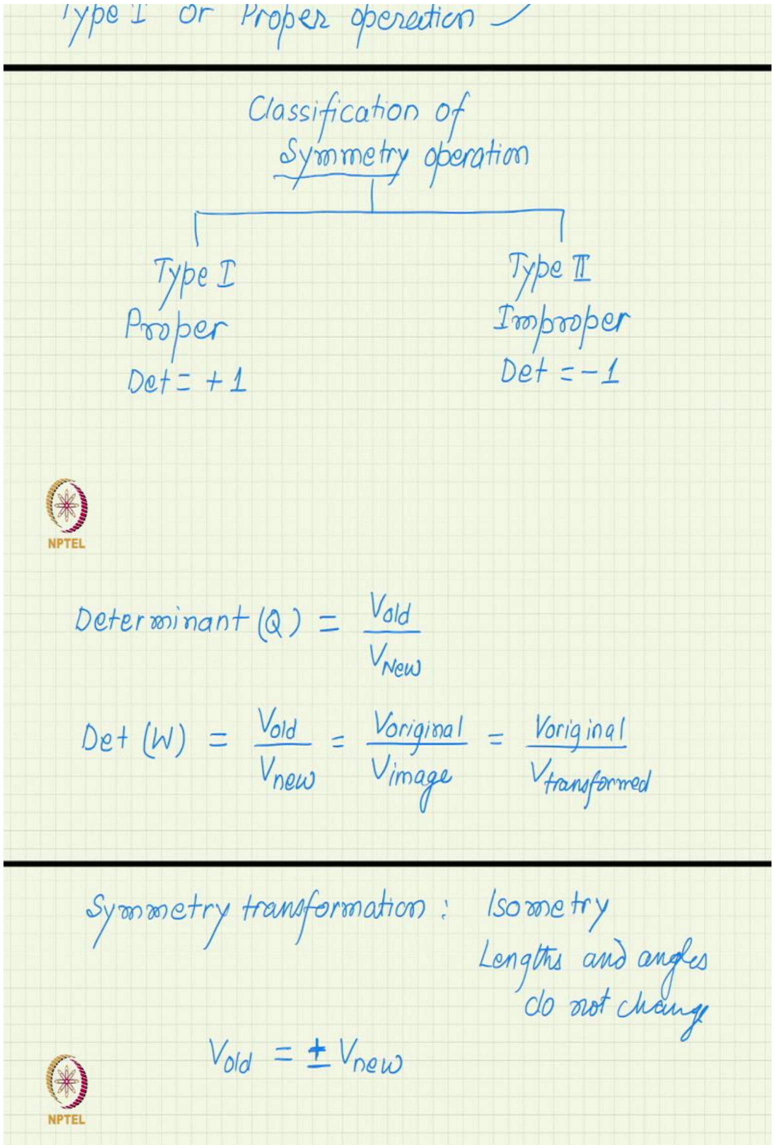

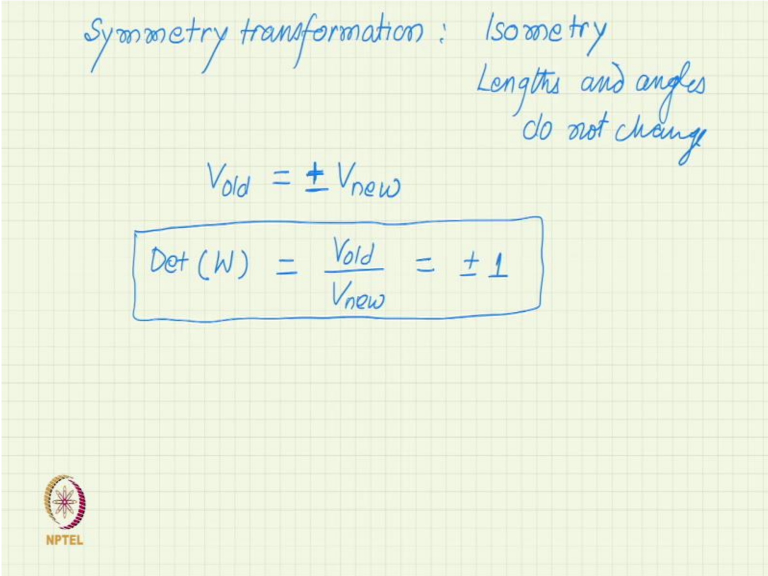

So, means essentially we have introduced the classification the various kinds of classification this is one classification of symmetry operation Type I, Type II Proper Improper I do not like read in proper. But that is how it is, it is like you are even an odd there is nothing odd about the poor odd numbers, they just number but historically, they are called odd numbers. So, historically these are called improper operations.

So, the determinant will always be plus 1, this we have not proved but if you reflect upon it, it will become clear that not only it will have a positive determinant, that positive value will always be plus 1, and determinant will be negative or minus 1 this is for symmetry operation. If it was not a symmetry operation, then also it can be a proper and improper operation in which case determinant will be positive.

But different from 1 and negative but different from 1 but if it is symmetry operation, it has to be plus 1 or minus 1 this is an application of what we learn when we were talking about the determinant in connection with coordinate transformation. So, where we, there we said the determinant of a coordinate transformation matrix that determinant of Q, determinant Q was V old by V New exactly the same argument is there for determinant of W also is V old by V new.

Student: Sir student (())(13:16) original by the (())(13:18).

Professor: You can call it if you want old is original, V original and new is the image of the original or transformed original you can call it V image. But in the last class, we saw that symmetry transformation is an isometry. What does that mean?

Student: The length do not change (())(14:06) change.

Professor: Symmetry transformation is an example of an isometry. So, length and angle do not change,if length and angles do not change, then what can you say about the old volume and the new volume.

Student: Amplitude or the magnitude of the volume.

Professor: Sorry.

Student: Amplitude or the magnitude of the volume will not see.

Professor: Amplitude or the magnitude of the volume will not see which all lengths are the same all angles are the same? So, volume of the unit cell box cannot change only unit cell box or the unit cell parallel piped is being transformed in space. If you are rotating it, it was here. Now it is got rotated there. If you are reflecting it, it was here and it has got reflected there. But since its edge lengths cannot change and since the angles between its edge length do not change.

So, even if you think in terms of that vector formula a dot b cross c, the triple product the volume is not going to change. So, isometry so, V old has to be equal to V new only, as we saw that if it is reflection the volume is having a negative sign, if it is a reflection the new volume will have a negative sign. So, it will be either plus or minus because determinant is changing because a right handed system changes into left handed system.

So, a dot b cross c if it is positive for a right handed system, it will become a negative for left handed system so, that clearly shows that determinant W if it is a symmetry operation has to be plus minus 1. So, this is an interesting result and we have to keep in mind. It is also a check it is also a check whether you after you have written your symmetry operation, whether you have not made any numerical mistake or so, so, if you calculate the determinant if it comes any different from either plus 1 or minus 1, whatever it may be, it is not a symmetry operation.