Crystals, Symmetry and Tensors Professor Rajesh Prasad Department of Materials Science and Engineering. Indian Institute of Technology Delhi 2-fold roto-inversion is a Mirror: Proof using Matrix Method

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Let us do another analytical proof that will come from the matrix method because we have to keep getting familiar with the matrix method also, because later on in the analysis of symmetry or if you write a computer programme to do any of these calculations, you cannot do it geometrically you have to do it by the matrix method. So, 2-fold roto-inversion. So, let us select the I itself as well origin.

So, I is the origin and let us choose x and y axis in the plane perpendicular to the axis and z parallel to the axis, this is the requirement and this is the limitation of matrix method because in matrix method, matrix is always with reference to some axis. See, geometrically when I was doing and I told you that 2 bar is m, I did not need x, y and z axis, I only needed the axis and the centre and the mirror plane.

But now, if you want to write a matrix for the symmetry operation, you require where is the origin and what are the axis. So, this is a convenient set of axis for 2-fold roto inverses. So, the first step is 2-fold rotation. So, let us say that the matrix for 2-fold rotation W2. How do you write? What will be W2? What will be the first column of 2-fold rotation? Minus 1, 0, 0.

Very good. Now, you really did not need that cos theta sine theta formula although that that works as you can see, because what was the first column supposed to be the transformation of

the first basis vector? What was the first basis vector that was a unit vector here e1 which was 1, 0, 0. If you rotate by 120-degree about z what happens to this after rotation it becomes minus 1, 0, 0. And that is what you write, the first column is the transformed first basis vector.

So, 1, 0, 0 becomes minus 180-degree rotation. So, that is the first column what is the second column? Now, you should be able to say quickly. So, that what you do to the y axis what you do to 0, 1, 0. So, what does the symmetry do to 0, 1, 0 it makes it 0 minus 1, 0 and what about the third axis that is the invariant axis remains 0, 0, 1.

So, this becomes my nice matrix for a 2-fold rotation. Now, but if it was a 2-foldrotation the matrix was complete, but I want to find matrix for 2-fold roto-inversion.

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inversion matrix $W_{i} = \begin{pmatrix} \overline{1} & 0 & 0 \\ 0 & \overline{1} & 0 \\ 0 & 0 & \overline{1} \end{pmatrix}$ 2- fold roto invension 2-fold rotation "followed" by inversion $\begin{pmatrix}
1 & 0 & 0 \\
0 & 1 & 0 \\
0 & 0 & 7
\end{pmatrix}$ $W_{\overline{2}} = W_i W_2 =$ 010 (1001)



So, I have to have a matrix for inverse and also. Who tell me the inversion matrix? What will inversion do to e1? What will inversion due to e1, if you invert. This pen in the centre inversion maps every point to 180-degree opposite point through the centre. So, 1 0 0 will become minus 1, 0, 0. 0, 1, 0 will become 0 minus 1, 0 and 0, 0, 1 will become 0, 0 minus 1 that it.

So, you can see the slight difference between a 2-fold rotation and the inversion, the first two columns are the same the third column 2-fold roto-inversion the axis was unchanged. So, it remained 0, 0, 1 for 2-fold, but in inversion the z axis also goes to minus z axis. So, 0, 0, 1 becomes 0, 0 minus 1. So, that is the inverse and matrix.

Now, 2-fold roto-inversion, this means inversion followed by a 2-fold rotation followed by inversion the geometrical operation of followed by is equivalent in matrix language multiplied by matrix multiplication of the matrix. So, inversion follows rotation. So, inversion matrix and a 2-fold matrix. So, W2 bar will be Wi into W2 you remember we always write the first matrix on the right and the second matrix on the left.

And if there was a third matrix then still on the left because what is the purpose of these matrices transform some vector, I want the image of some vector by multiplying it by matrix. So, if I multiply a vector with this product, which matrix will act first on it with W2. So, the first matrix is always written on the left. So, what do you find if you now use the result now, interpret this matrix. So, this is the 2-fold roto-inversion axis.

Now, if I again interpret in the same way the first column was telling me what happens to 1, 0, 0. So, nothing happens to 1, 0, 0. So, this matrix leaves 1, 0, 0 unchanged. 1, 0, 0 remains where it was because the first column is 1, 0, 0. The second column remains unchanged. So, 0, 1, 0 remains where it was, but the third column which was 0, 0, 1 becomes 0, 0 minus 1 which operation will do that reflection in the plane.

So, this is equivalent to mirror in the, you can say 0, 0, 1 plane passing through the origin. So, that is a matrix way of seeing that a 2-fold roto-inversion is nothing but a mirror plane perpendicular to the rotation axis.