CRYSTAL SYMMETRY, X-RAY DIFFRACTION, AND PHYSICAL PROPERTIES

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Lecture 37: Space Groups: Screw Axes

So, in this lecture we are going to discuss the screw axis in detail. In the previous lecture, I had briefly introduced the concept of a screw axis while developing certain space groups. Towards the end of that lecture, I added a twofold screw axis to a primitive monoclinic lattice. In that particular space group, the symbol for the screw axis appears because all the twofold rotational symmetries that would normally be pure twofold rotations have been replaced by screw axes.

In this lecture, we will discuss the meaning of the symbol 2_1, and we will also see that there are other screw axes, such as threefold and fourfold screw axes, which are represented using different symbols. For the purpose of comparison, let us first consider a pure twofold rotational axis.

Suppose we have a pure twofold rotational axis, represented by the black line shown here. If we place a motif at this position, a rotation of 180° will take this motif to this position. If $\bar{t}$ denotes a lattice translation along the axis, then both of these motifs will be translated along the axis by $\bar{t}$, and this process can be continued indefinitely. This is simply the pattern corresponding to a pure twofold rotational symmetry.

Now, let us consider a twofold screw axis, denoted by 2_1. As mentioned earlier, this operation consists of a twofold rotation, that is, a rotation of 180°, followed by a translation. Let us denote the translation by τ. The question is, how large should this translation be? In this case, the translation is exactly half of the lattice translation along the screw axis. Here, t denotes the lattice translation along the screw axis.

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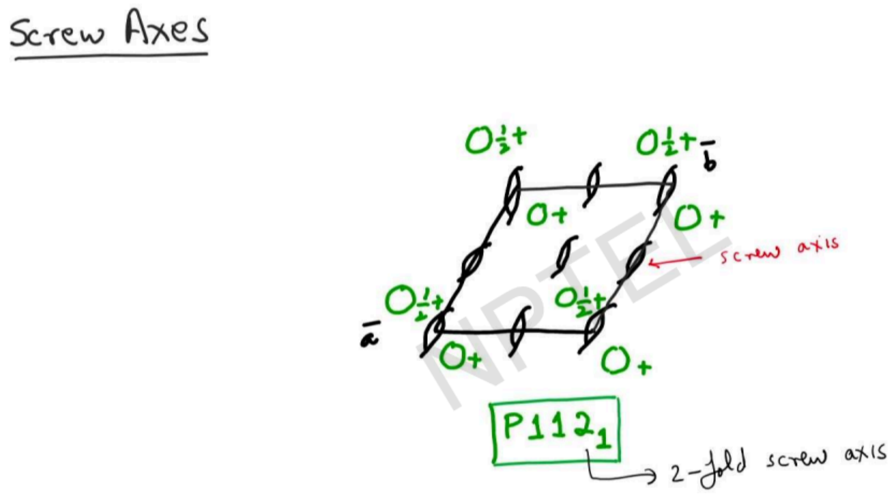

We now place a motif at this position and label it as motif number 1. We rotate it by 180°, which would bring it to this position, and then we translate it upward by half the lattice translation, that is, by $\bar{t}/2$. The motif therefore appears at this new position. The intermediate position where the rotated motif was drawn must be removed, because the motif does not remain there. The operation is strictly a 180° rotation followed by a translation of $\bar{t}/2$.

Thus, any screw axis is a two-step operation, similar to a glide plane. In the case of a glide plane, we have a reflection followed by a translation parallel to the plane. In the case of a screw axis, we have a rotation followed by a translation parallel to the axis. Through this operation, motif number 1 is transformed into motif number 2. Applying the same operation again, another 180° rotation followed by a translation of $\bar{t}/2$ generates motif number 3. Repeating this process generates motif number 4, then motif number 5, and so on.

This is the type of pattern that is generated along the screw axis for a twofold screw axis represented by the symbol 2_1. If we examine the relationship between motif numbers 1 and 3, we can easily see that they are related by a simple lattice translation. Similarly, motifs 3 and 5 are related by a lattice translation, and motifs 2 and 4 are also related by a lattice translation. This pattern is therefore different from the pattern obtained in the case of a pure twofold rotational symmetry.

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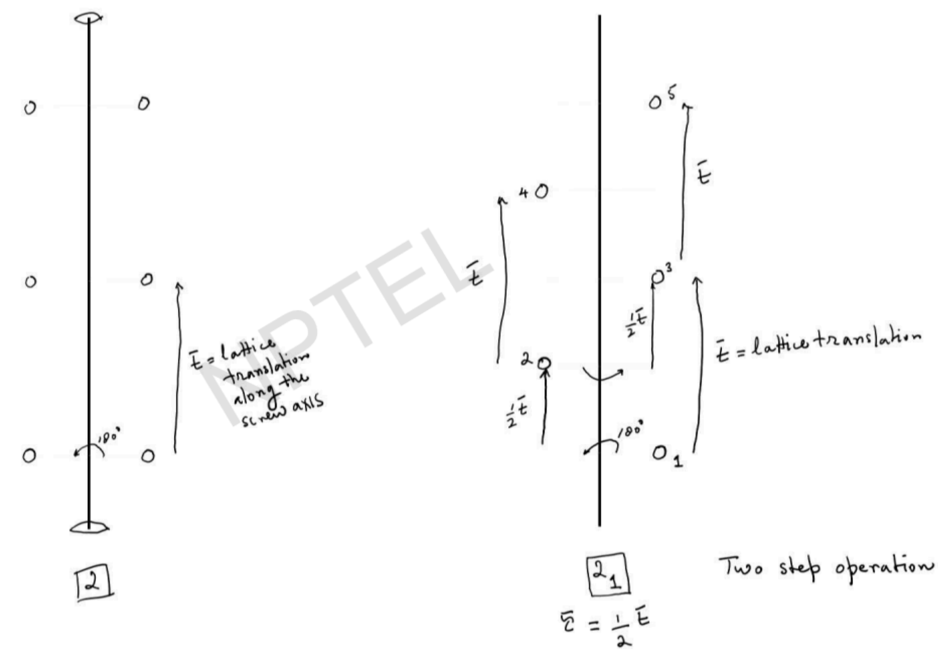

Let us now move on to higher-order screw axes, such as those associated with threefold rotational symmetry. First, consider a pure threefold rotational axis. If we place a motif at some position, a rotation of 120° about the axis will take the motif to a second position. Another 120° rotation will move it to a third position, and a further 120° rotation will bring it back to the original position. If we now assume that $\bar{t}$ is a lattice translation along the axis, then all three motifs will be translated by $\bar{t}$, producing the expected pattern for a pure threefold rotational symmetry.

Now, just as we had a symbol 2_1 for the twofold screw axis, we can introduce symbols for threefold screw axes. One such symbol is 3_1, but we will find that there is more than one possible screw axis associated with threefold symmetry. In particular, we can have 3_1 and 3_2. The difference between these lies in the magnitude of the translation along the screw axis.

For the 3_1 screw axis, the translation τ is one-third of the lattice translation $\bar{t}$. For the 3_2 screw axis, the translation is two-thirds of the lattice translation $\bar{t}$, where $\bar{t}$ is the lattice translation along the screw axis.

Let us first consider the 3_1 screw axis. We place a motif at this position and label it as motif number 1. We rotate it by 120°, bringing it to a new angular position, and then translate it upward by $\bar{t}/3$. This generates motif number 2. Applying another 120° rotation followed by a translation of $\bar{t}/3$ generates motif number 3. Repeating this sequence produces motif number 4, then motif number 5, then motif number 6, and finally motif number 7.

This is the pattern obtained for a threefold screw axis with a translation vector of $\bar{t}/3$. If we examine the pattern carefully, we see that the translation from motif 1 to motif 4 corresponds to a full lattice translation $\bar{t}$, since it involves three successive translations of $\bar{t}/3$. Similarly, motifs 4 and 7 are related by a lattice translation. If we look at motifs 2 and 5, they are also related by a lattice translation, and the same applies to other sets of motifs. Thus, many motifs in this pattern are related by lattice translations. This is the characteristic pattern for the 3_1 screw axis.

Now, let us consider the second threefold screw axis, 3_2. In this case, the screw translation is $2\bar{t}/3$. Starting again with motif number 1, we rotate it by 120°, and instead of moving it upward by $\bar{t}/3$, we move it upward by $2\bar{t}/3$. This displacement can be visualized as two successive translations of $\bar{t}/3$. The motif therefore reaches position 2. Applying another 120° rotation followed by a translation of $2\bar{t}/3$ generates motif number 3. A further 120° rotation and a translation of $2\bar{t}/3$ generates motif number 4.

At this stage, we may not immediately see motifs that are directly related by a lattice translation. However, lattice translations are always present in the crystal. We can therefore introduce the lattice translation explicitly. Starting from motif number 1, if we apply three successive translations of $\bar{t}/3$, we obtain a full lattice translation $\bar{t}$, which brings us to motif number 5. Similarly, motif number 5 can be related to motif number 4 by another lattice translation. If we start from motif number 2 and apply three successive translations of $\bar{t}/3$, we obtain motif number 6. Starting from motif number 3 and applying three successive translations of $\bar{t}/3$, we obtain motif number 7.

This completes the pattern for the 3_2 screw axis. Now, let us compare the 3_1 and 3_2 screw axes. For the 3_1 screw axis, each 120° rotation is followed by a translation of $\bar{t}/3$. Thus, as the motif rotates around the axis, it moves upward along the axis, and the successive positions can be connected by a helical path.

For the 3_2 screw axis, we can also view the motion in a reverse manner. For example, to go from motif number 4 to motif number 6, we rotate by 120° and translate by $-\bar{t}/3$. Similarly, to go from motif number 6 to motif number 3, we rotate by 120° and translate again by $-\bar{t}/3$. Continuing this process, we see that repeated operations cause the motif to move downward along the screw axis. In this way, the helical nature of the screw axis becomes evident.

So, in one case, in 3_1, when the same rotation is applied, the motion proceeds upward along the screw axis, whereas in the other case it proceeds downward along the screw axis. In other words, the two screw axes have helical paths that are opposite to each other. One way to interpret this is to call one a right-handed screw and the other a left-handed screw. Thus, for the threefold case, there are two distinct screw axes.

Now, let us consider a screw axis with fourfold rotation, that is, a 90° rotation. As before, we first construct the pattern for a pure fourfold rotational symmetry. Starting with a motif, we rotate it by 90°, then by another 90°, and then by another 90°, after which a lattice translation is applied. This produces the pattern corresponding to a pure fourfold rotation symmetry, where t denotes the lattice translation.

In this case, there are three different screw axes. These are denoted as 4_1, 4_2, and 4_3. It is possible to anticipate the translations involved in the operation of these three screw axes. For 4_1, the screw translation τ is $\frac{1}{4}\bar{t}$. For 4_2, τ is $\frac{2}{4}\bar{t}$, which is simply $\frac{1}{2}\bar{t}$. For 4_3, τ is $\frac{3}{4}\bar{t}$

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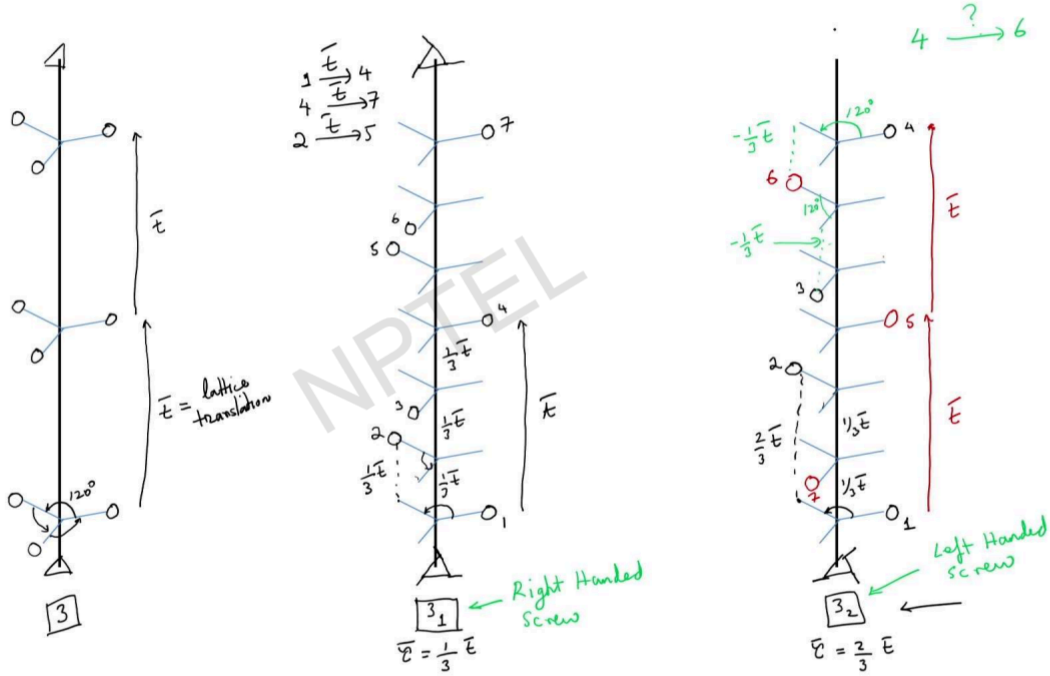

Let us begin with 4_1. We start with motif number 1. A rotation of 90° followed by a translation of $\frac{1}{4}\bar{t}$ brings us to motif number 2. Another 90° rotation followed by the same translation brings us to motif number 3. Repeating this process brings us successively to motifs 4, 5, 6, and finally motif number 7. This constitutes the complete pattern for the 4_1 screw axis.

Within this pattern, lattice translations can be identified. For example, to go from motif number 3 to motif number 7, we apply four successive translations of $\frac{1}{4}\bar{t}$, which together give a full lattice translation $\bar{t}$. Hence, motifs 3 and 7 are related by a lattice translation. Similarly, motifs 2 and 6 are related by a lattice translation, and motifs 1 and 5 are also related by a lattice translation. This describes the characteristic pattern for the 4_1 screw axis.

Before discussing 4_2, let us examine the screw axis 4_3. In this case, the screw translation is $\frac{3}{4}\bar{t}$. We again begin with motif number 1. After a 90° rotation, we translate by three quarters of the lattice translation, that is, $\frac{3}{4}\bar{t}$. This can be visualized as three successive steps of $\frac{1}{4}\bar{t}$. This operation brings us to motif number 2. Applying another 90° rotation followed by the same translation brings us to motif number 3.

Now, we also apply lattice translations to this pattern. For example, starting from motif number 3, a lattice translation of $\bar{t}$ moves it to motif number 4. Similarly, starting from motif number 1, a lattice translation of $\bar{t}$ moves it to motif number 5. Thus, motifs 3 and 4 are related by a lattice translation, as are motifs 1 and 5.

As in the earlier discussion of 3_1 and 3_2, the screw translation can also be considered in the opposite direction. For example, to go from motif number 5 to motif number 2, we rotate by 90° and then translate by $-\frac{1}{4}\bar{t}$. That is, we apply a rotation of $\pi/2$ followed by a screw translation of $-\frac{1}{4}\bar{t}$. This operation is valid for a screw axis whose positive translation is $\frac{3}{4}\bar{t}$. Thus, we can take motif number 3, rotate it by 90°, and then move downward by $-\frac{1}{4}\bar{t}$ to obtain a new motif, which we label as motif number 6. Applying a lattice translation to motif number 6 then completes the pattern for the 4_3 screw axis.

As can be seen, this situation is very similar to the earlier case of 3_1 and 3_2. In 3_1, the rotation is accompanied by motion upward along the axis, whereas in 3_2, the rotation is accompanied by motion in the opposite direction by the same amount of $\frac{1}{3}\bar{t}$. Similarly, in the fourfold case, 4_1 corresponds to motion in one direction along the axis, while 4_3 corresponds to motion in the opposite direction. One may loosely describe one as right-handed and the other as left-handed. However, this terminology does not imply chirality, since there is no change in the handedness of the motifs themselves. The terms are used only to describe the sense of the helical motion.

Now, let us consider the third screw axis, 4_2. Starting with motif number 1, we rotate by 90° and then translate by $\frac{1}{2}\bar{t}$. This brings us to motif number 2. Another 90° rotation followed by a translation of $\frac{1}{2}\bar{t}$ brings us to motif number 3. Lattice translations can also be applied. For example, applying a lattice translation $\bar{t}$ to motif number 3 brings it to motif number 4, and applying a lattice translation to motif number 1 brings it to motif number 5.

Next, we take motif number 3, rotate it by 90°, and then translate downward by $-\frac{1}{4}\bar{t}$, which brings us to motif number 6. An interesting feature of this pattern is that it clearly exhibits a pure twofold rotational symmetry. This indicates that the 4_2 screw axis contains, as a subset, a pure twofold rotation.

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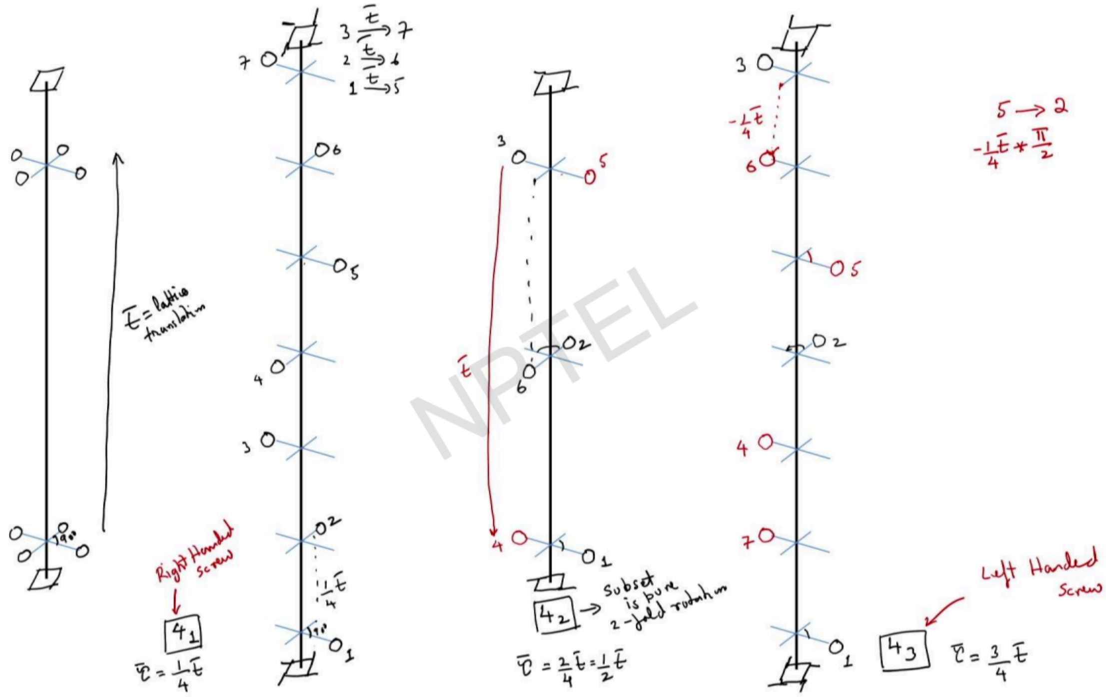

Before concluding the lecture, let us summarize the graphical symbols used for screw axes. The symbol for 2_1 is the one we have already seen. For 3_1, the triangle is drawn first, and fins are added in a particular orientation. For 3_2, the fins are drawn in the opposite orientation, distinguishing it from 3_1. Similarly, for 4_1 and 4_3, the graphical symbols are related by reversing the orientation. In the case of 4_2, the symbol itself clearly shows a twofold rotational symmetry as a subset.

With this, I conclude the lecture on screw axis symmetry. Thank you.