CRYSTAL SYMMETRY, X-RAY DIFFRACTION, AND PHYSICAL PROPERTIES

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Lecture 38: Space Groups: Glide Planes

In the last lecture, we had some discussion on the screw axis. In today's lecture, we will examine glide planes in three-dimensional space lattices. In an earlier lecture, we introduced a glide plane of the following type, where the glide is represented by a symbol that starts like a mirror, and an arrow indicates the glide direction. In this case, the arrow indicates that the glide direction is along the $\bar{b}$ direction, and since $\bar{b}$ is a lattice translation, the glide magnitude must be $\frac{\bar{b}}{2}$. This particular space group was referred to as $P11b$.

Let us now consider this in more detail by taking a different case. Assume that we have orthogonal axes $\bar{a}$, $\bar{b}$, and $\bar{c}$, where $\bar{a}$ and $\bar{b}$ lie in the plane, and $\bar{c}$ is normal to the AB plane. We consider a b glide indicated by the same symbol. This is referred to as a b glide, indicating that the glide direction is along $\bar{b}$. If a motif is placed at a point above the plane, the glide plane reflects this motif below the AB plane, changes its handedness, and then translates it by $\frac{\bar{b}}{2}$ to bring it to a new position. The change in handedness is indicated, and the motif is marked with a minus sign to show that it has gone below the AB plane. Reflecting again and applying another glide translation of $\frac{\bar{b}}{2}$ brings the motif to another position. These two motifs are related through a lattice translation $\bar{b}$. A lattice translation along $\bar{a}$ will generate the full pattern by bringing all these motifs to equivalent positions.

This figure can be understood as a projection along the c axis. In this representation, the projection direction is along $\bar{c}$, and the glide translation vector is $\tau = \frac{\bar{b}}{2}$.

Now consider the same b-glide, but change the projection axis. Let us take a projection along $\overline{a}$. In this case, the axes in the plane are $\overline{b}$ and $\overline{c}$, and the a axis comes out of the plane. The origin remains the same, and the $\overline{a}$ vector is normal to the BC plane. Although we are viewing the system from a different orientation, the glide remains a b-glide. The glide plane is still the AB plane. Since the AB plane is now perpendicular to the BC plane, the glide plane itself is perpendicular to the plane of the figure and parallel to AB. Consequently, the glide plane is indicated as being perpendicular to the figure.

In this view, the glide is represented by a dashed line. This is the same graphical representation used for glide lines in plane groups, where the glide appears in only one orientation. The dashed line indicates that the glide plane is perpendicular to the BC plane, and the glide direction is along $\overline{b}$. The glide direction is shown accordingly. Placing a motif above the glide plane, reflecting it across the plane, and translating it by $\frac{\overline{b}}{2}$ leaves it above the plane. Repeating the reflection and translation again changes the handedness once more. If we label these motifs as 1, 2, and 3, then 1 goes to 2 with a handedness change, 2 goes to 3 with another handedness change, and 1 can also go to 3 through a lattice translation of $\overline{b}$. This demonstrates how the same space group appears in this projection.

Let us now take another view by choosing a projection along $\overline{b}$. In the first case, the projection was along $\overline{c}$, and in the second case it was along $\overline{a}$. For the third diagram, we must ensure that the axes are correctly oriented. Here, the axes are $\overline{c}$ and $\overline{a}$ in the plane, with the origin defined accordingly. It is important to note that, even in the previous cases, we are following a right-handed coordinate system, and this same system must be maintained. With $\overline{b}$ coming out of the plane, $\overline{c}$ and $\overline{a}$ remain in the plane, and the orientation is consistent.

The glide plane is still the AB plane. Since the b axis is coming out of the plane and the a axis lies in the plane, the glide plane is perpendicular to the AC plane. Thus, the glide plane is perpendicular to the plane of the figure. The glide translation is along $\overline{b}$, and since $\overline{b}$ is normal to the figure, the glide translation is also normal to the figure. In this case, the glide plane is indicated by a dotted line. The dotted line signifies that the glide plane is perpendicular to the AC plane, and the glide translation vector τ is perpendicular to the AC plane and directed along the b axis.

If we now place a motif above the AC plane, it is reflected through the glide plane and then translated along $\overline{b}$, which means it moves upward. This is indicated by a change in handedness and a displacement upward by half the lattice translation, that is, by $\frac{\overline{b}}{2}$. Lattice translations then generate equivalent motifs. All three diagrams described so far represent the same glide plane in the same space group, but shown from different perspectives. Understanding these perspectives is essential for correctly reading the International Tables.

In the same way that we have discussed a b-glide, we can also have an a glide, where the glide direction is along a, or a c-glide, where the glide direction is along $\overline{c}$. As an exercise, one can attempt to draw the corresponding sketches for a and c-glides.

In addition, there is a diagonal glide, known as an n glide. In this case, the glide translation is along the diagonal of the AB plane. The glide translation vector is therefore $\frac{\overline{a}}{2} + \frac{\overline{b}}{2}$, and the glide plane itself is the AB plane. If a motif is placed above the plane, it is reflected below the plane and then translated along the direction $\frac{\overline{a}}{2} + \frac{\overline{b}}{2}$. This brings the motif to a new position with changed handedness below the plane, which is indicated by a minus sign. This description corresponds to a projection along C.

Now consider a projection along $\overline{b}$ for the same diagonal glide. In this case, the plane of the figure is the AC plane, and the $\overline{b}$ vector is normal to it. The glide plane is the AB plane, which means that the glide plane is perpendicular to the AC plane. The glide direction $\tau = \frac{\bar{a}}{2} + \frac{\bar{b}}{2}$ remains the same, but we are now viewing it from a different perspective. The glide direction is neither perpendicular nor parallel to the AC plane; instead, it lies at an oblique angle. To represent this situation graphically, the glide plane is drawn using a combination of dashes and dots. This symbol indicates that the glide direction is neither parallel nor perpendicular to the plane of projection.

Placing a motif in this configuration, reflecting it across the glide plane, and translating it by $\frac{\bar{a}}{2} + \frac{\bar{b}}{2}$ moves it to a new position with changed handedness. Repeating the operation generates the full pattern. In all these cases, the glide plane remains parallel to the AB plane.

Finally, consider another type of glide known as the diamond glide, or d glide. In this case, the glide plane is parallel to the BC plane, which means it is perpendicular to the AB plane. The glide translation vector is $\tau = \frac{\bar{b}}{4} + \frac{\bar{c}}{4}$. This glide is represented graphically using a combination of arrows and dots. If a motif is placed above the glide plane, it is reflected and then translated by $\frac{\bar{b}}{4}$ horizontally and $\frac{\bar{c}}{4}$ vertically upward. The handedness changes, and the motif moves upward by one quarter of the lattice translation. Reflecting again changes the handedness once more and adds another quarter translation, bringing the motif to the half position. Continuing this process generates the full pattern produced by the diamond glide.

This provides a summary of all the glide planes that we will encounter. We now consider a few additional examples of space groups. In an earlier lecture, we discussed the space group $P112_1$, where $\bar{a}$ and $\bar{b}$ lie in the plane and the c axis is the unique axis. In this case, the 2_1 screw axis is parallel to the c axis, making c the unique axis.

Often in monoclinic space groups, the b axis is chosen as the unique axis. If we make this choice, the same space group symbol $P112_1$, where $\bar{c}$ is the unique axis, becomes $P12_11$

when $\overline{b}$ is taken as the unique axis. In this setting, the 2_1 screw axis is parallel to $\overline{b}$. Here, $\overline{c}$ and $\overline{a}$ lie in the plane, and the b axis is perpendicular to the AC plane. The resulting

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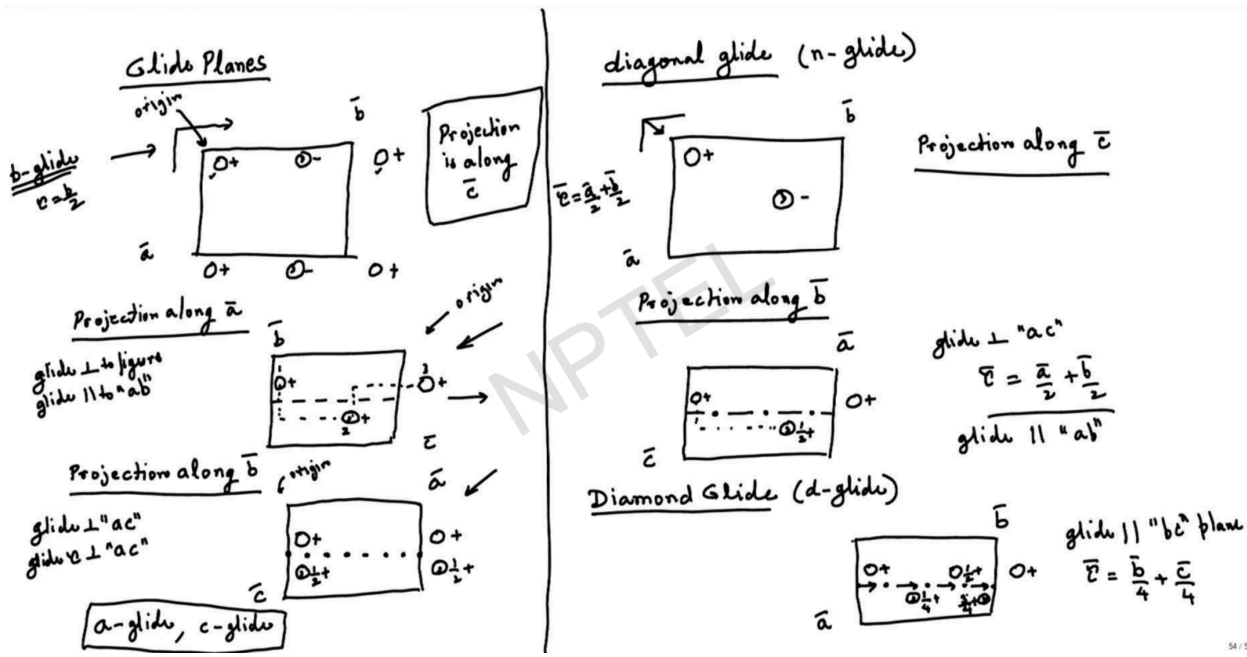

diagram is equivalent to the one drawn earlier, with the 2_1 screw axes distributed throughout the unit cell. A motif placed in the cell is rotated by the screw axis and translated by half a lattice translation, and lattice translations generate the full pattern. Motifs related by the central 2_1 screw axis can be clearly identified.

This configuration corresponds to the space group $P12_11$ with the b axis as the unique axis. Now consider a different orientation. Since b is perpendicular, both the bc plane and the ab plane are rectangles. Let us take a projection such that the bc plane is projected, that is, a projection along $\overline{a}$. In this case, the b axis lies in the plane, and the c axis is projected at an angle to $\overline{a}$, resulting in a projected length denoted as $\overline{c}_p$, where the subscript p indicates projection along $\overline{a}$.

The 2_1 screw axis is parallel to the $\overline{b}$ vector and therefore lies in the plane of the figure. It is represented accordingly, with three screw axes appearing in the plane: along the edges and at the center. If a motif is placed, it is rotated by 180° and then translated by $\frac{\overline{b}}{2}$. The 180° rotation moves it below the plane without changing handedness, and the translation shifts it upward. Repeating the operation and applying lattice translations generates the full pattern. This is again the same space group $P12_11$, shown from a different viewpoint. In the previous case, the projection axis was $\overline{b}$, whereas here the projection axis is $\overline{a}$.

Next, consider the space group $P1c1$. This is again a primitive monoclinic space group, where c denotes a c-glide, meaning that the glide direction is along $\overline{c}$. The b axis is again the unique axis. When the projection axis is $\overline{b}$, the c glide is perpendicular to $\overline{b}$. In this view, $\overline{c}$ and $\overline{a}$ lie in the plane, and $\overline{b}$ is perpendicular to the AC plane. The c-glide is represented as a mirror with an arrow indicating translation along $\overline{c}$. Placing motifs and applying glide reflections and translations by $\frac{\overline{c}}{2}$ generates the space group pattern.

Now consider a projection along $\overline{a}$. In this case, the $\overline{b}$ vector lies in the plane, the $\overline{c}$ vector is projected, and the origin is defined accordingly. The glide plane is parallel to the AC plane, and since $\overline{a}$ comes out of the plane, the glide plane is indicated appropriately. The glide translation is along $\overline{c}$. The motifs can be filled in straightforwardly in this view.

Finally, consider a projection along $\overline{c}$. Since $\overline{a}$ and $\overline{c}$ do not make a 90° angle, the projection of $\overline{a}$ has a reduced length, which we denote as $\overline{a}_p$. The glide plane is parallel to the AC plane, and the $\overline{c}$ axis comes out of the plane. The glide direction is also along $\overline{c}$. In this case, the glide is indicated by a dotted line. The motifs can again be filled in accordingly.

With this discussion of glide planes, together with the previous lecture on screw axes, we conclude this topic. In the next lecture, we will revisit the International Tables. We have already examined the International Tables for plane groups; next, we will study the International Tables for space groups. Thank you.

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