

CRYSTAL SYMMETRY, X-RAY DIFFRACTION, AND PHYSICAL PROPERTIES

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Lecture 03: Crystallographic Patterns

Continuing from the last lecture, let us take another look at this two-dimensional crystal. We have a lattice whose translation vectors are \bar{a} and \bar{b} . In this crystal, let us consider an atom, which we will call atom A, and let us place it so that its center coincides with a lattice point. Now, how can we describe this crystal structure?

The standard way is to describe the lattice first. The lattice is specified by the vectors A and B, and the motif gives the position of the atom with respect to each lattice point.

In this case, the position of atom A is at (0, 0).

What this means is that we draw a vector from each lattice point to the position specified in the motif, which in this case is (0, 0). This essentially means that the atom is placed directly on the lattice point. Now, imagine that we have another atom, which we will call atom B, whose position is at some coordinates (x, y) with respect to each lattice point.

What this means is that the coordinates (x, y) could correspond to some point here.

Essentially, we draw a vector from each lattice point to the position (x, y), and we do this for every lattice point. This is how atom B is positioned in the crystal. The same vector is drawn from each lattice point, so there is no ambiguity. Thus, atom A is located at (0, 0) with respect to each lattice point, and atom B is located at (x, y) with respect to each lattice point.

Now, just as we have a unit cell for the lattice, we use the same unit cell for the crystal.

This unit cell is defined by the vectors \bar{a} and \bar{b} . If we examine it, this was a primitive cell

for the lattice, and it remains a primitive cell for the crystal because it still contains one lattice point per unit cell. However, now we must ask: how many atoms are present within this unit cell?

If the motif consists of only one atom, then clearly the atom A, located at the corners of the unit cell, is shared by four adjacent unit cells. Thus, only one-fourth of atom A belongs to this unit cell. Since there are four corner atoms, the total contribution from atom A is:

$$4 \times \frac{1}{4} = 1$$

So, there is one atom A per unit cell. Now, consider atom B. Out of the four B atoms, one atom is completely inside the unit cell. Hence, there is one atom B per unit cell. Therefore, the total number of atoms in the unit cell is two: one A atom and one B atom.

Now, if we want to determine the lattice parameters of the unit cell, how many are required to define it? We need the magnitudes of the vectors \vec{a} and \vec{b} , and we also need to know the angle between the two vectors, which we can denote as α . Thus, there are a total of three lattice parameters for the unit cell: a , b , and α . By defining these parameters, we fully describe the unit cell of the lattice, which then becomes the unit cell for the crystal structure once the motif is added to the lattice points.

Now, just one point to note is that the motif can be replaced by literally anything. For example, consider a lattice of points, and let us choose a very different kind of motif, not an atom. Suppose we take a motif in the shape of the letter L, with some coordinates (x, y) for this symbol. This motif could be positioned, for instance, at the coordinates (x, y) within the unit cell.

So, instead of atoms, we now have a pattern, represented by this particular symbol. One can create any other pattern as well. For example, if we take a different shape or symbol,

we can populate this motif at all the lattice points. The location I have chosen here serves as the reference point, from which the (x, y) coordinates of the motif are measured.

So, in this case, the motif is at coordinates (x, y) , and we draw vectors from each lattice point to position the motif at every lattice point. Essentially, what we have done is create a repeating pattern using this motif at all lattice points. In particular, these are examples of crystallographic patterns. Thus, in essence, crystallography is the study of such ordered arrangements of motifs on a lattice.

Crystallography is a study of patterns, and by studying these patterns we are also understanding the development of crystals where atoms are present. Many times, by using these patterns, they are useful to understand crystallography in better detail, as we will see later on in the course.

For example, if we look at the first pattern, we could create a motif with two entities. Let us say the first entity is located at (x_1, y_1) , and the second entity is located at (x_2, y_2) .

We then draw a vector to (x_2, y_2) and place the second element of the motif at that position for each lattice point.

So, in this case, I have created a different kind of pattern. How is it different? Let us try to understand this, though we will delve into greater detail later. So far, we have only considered translation symmetry, but there are other symmetry elements that also play a role. For instance, if we now look at the same lattice, we can draw a separate figure to illustrate this.

One of the symmetry elements that we will examine, among others, is reflection symmetry. If we draw a line, this line represents a mirror plane. As can be seen, this

This is important to understand because many misconceptions arise from this, as we will see. In actual crystallography, it is the study of patterns, and now we want to extend the idea of a lattice and a crystal to three dimensions. Let us, therefore, examine the lattice in three dimensions.

So, for a lattice in three dimensions, let us understand what kind of unit cell we have. Since it is difficult to draw the lattice points in three dimensions, we will consider it from the perspective of the unit cell.

In two dimensions, all unit cells are some form of parallelogram, some may be very oblique, while others may resemble a square or a rectangle but they are all parallelograms. In three dimensions, the unit cell is called a parallelepiped. Let us consider this, and define the axes as x , y , and z . This represents a unit cell in three dimensions. Regarding the lattice parameters, just as we had a and b as lattice vectors in two dimensions, with the angle between them as α , we now have additional vectors and angles to define the three-dimensional unit cell.

Now, in three dimensions, we have many more lattice parameters. We have the lattice vector \bar{a} along the x -axis, vector \bar{b} along the y -axis, and vector \bar{c} along the z -axis. Thus, we have three length parameters, a , b , and c , instead of only two as in the two-dimensional case. In addition to the lengths, we also need to specify the angles between these vectors.

The angle between vectors b and c is called α , the angle between vectors c and a is called β , and the angle between vectors a and b is called γ . If you notice, these are the conventional parameters used to describe a three-dimensional unit cell.

So, the angle between b and c is α . You can see that we use Greek letters for the angles in the same order as the vectors a, b, c . The first three letters in English are a, b, c , and the corresponding Greek letters are α, β, γ . Between b and c , the missing vector is a , so we call the angle α . Between a and c , the missing vector is b , so the angle is β . Between a and b , the angle is γ . Thus, there are a total of six parameters: three length parameters a, b, c and three angle parameters α, β, γ .

Based on these parameters, we can construct different kinds of unit cells. We will now compare the unit cells in two dimensions with those in three dimensions, and later we will derive why these specific unit cells are defined.

Let us first consider two-dimensional unit cells. One type is called oblique, and all of them are parallelograms. The oblique cell is defined by a, b , and α . These are three independent parameters: a and b have no constraints, and α also has no constraints. Thus, a, b , and α can take any possible values.

A second lattice is called rectangular, or I should say actually I should add the word primitive as well. So, there would be primitive rectangular. The third one is called a centred rectangular unit cell or lattice. Fourth one is called square, primitive square, and fifth is hexagonal. I will come later as to what kind of constraints each one of the lattices put on the parameters a and b . Now, let us look at the three-dimensional unit cells.

Just before that primitive oblique obviously very clear all the lattice points are at the corners, primitive rectangular all the lattice points at the corners of a rectangle, centered rectangular means lattice points at the corner and one lattice point in the center, primitive square again only lattice points at the corners of the cell, hexagonal is also primitive. So, the lattice points only at the corners of the unit cell.

I am deliberately not trying to define these unit cells more than this. We will be coming to this pretty quickly in this course, where you will see how we define the lattices and what is the basis of defining the different lattices that we have. So, in three-dimensional unit cells: where can I put the lattice points on this parallelepiped?

Well, one place I can put lattice points is obviously the corners. By doing this, I am forming a primitive unit cell, and once I translate this unit cell by a in the x direction, b in the y direction, and c along the z direction, I will get the entire infinite lattice. So, that is one. I will form a primitive lattice. What else can I do? In addition to the lattice points only at corners, I can still have a valid lattice, which means it follows translation symmetry. So, in addition to lattice points at corners, I can add one lattice point at the body-centered position. So, I have lattice points at the corners, and I have one lattice point at the body-centered position.

Another alternative is lattice points at the corners plus centers of two opposite faces. A third option is lattice points at the centers of all six faces of the parallelepiped. So, what I have described right now are four different classifications: one, primitive, with lattice points only at the corners; two, body-centered, with lattice points at the corners plus one at the center; three, face-centered on two opposite faces, with lattice points at the corners plus centers of two opposite faces; and four, face-centered on all six faces, with lattice points at the corners plus centers of all six faces of the parallelepiped. You can clearly see that if I look at how many lattice points are there per unit cell, they will differ for each case.

Here, of course, in the primitive lattice, I will have only the corner lattice points, which effectively gives one lattice point per unit cell. In the body-centered lattice, I have one lattice point at the corners and one at the body-centered position, giving two lattice points per unit cell. For the lattice with centers of two opposite faces, let us say I put a lattice point on the top face and one on the bottom face. Each of these lattice points is shared by

two unit cells, so each contributes half to the unit cell. Adding the two contributions from the opposite faces gives one lattice point, and with the corner contribution, the total is two lattice points per unit cell.

If I look at the lattice points in this case, with six faces plus corners, then from each face I have half a lattice point, and there are six faces, then

$$6 \times \frac{1}{2} = 3$$

Adding from the corners, which is 1 lattice point, gives a total of 4 lattice points per unit cell. So, essentially, I have defined four classes, or four different ways to place lattice points without violating the lattice condition, which is that all lattice points must obey translation symmetry.

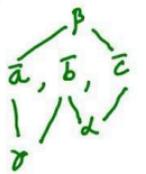
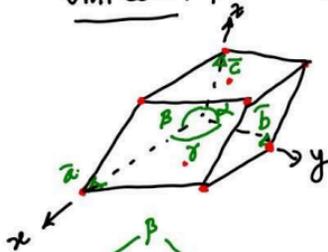
Finally, I will leave you with one question. Consider a unit cell. Consider this unit cell and let me put lattice points again at all the 8 corners, and I will put lattice points only, let us say, on this left face, on the right face, in the front face, and at the back face. Then, I have essentially put four additional lattice points on the vertical faces, and I have put no lattice point on the top face and the bottom face. So, I have essentially added corners plus four lattice points on the centers of vertical faces. Is this allowed?

Well, the answer is no to this because this will violate the translation symmetry or that every lattice point must have an identical environment as we had discussed in the last class and I will leave this to you to verify that this is indeed not a lattice.

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Lattice in 3D

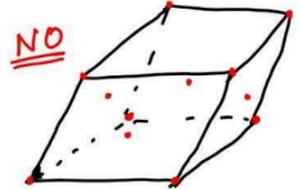
Unit cell: parallel piped



Six parameters

2D unit cells (a, b, alpha)

- Primitive
 1. Oblique $\rightarrow a \neq b$ (no constraints)
 2. Primitive Rectangular
 3. Centred Rectangular
 4. Primitive Square
 5. Hexagonal (Primitive)



Corners + 4 on centers of vertical faces

3D unit cells

- Primitive (lattice only at corners) $\rightarrow 1$

In addition to lattice pts at corners:

- Body centred position $\rightarrow 1+1=2$
- Centres of 2 opposite faces $1+1=2$
- Centres of all 6 faces $= 1+6 \times \frac{1}{2} = 4$