

CRYSTAL SYMMETRY, X-RAY DIFFRACTION, AND PHYSICAL PROPERTIES

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Lecture 12: 2D Crystal Systems and Lattices - I

We will start out today, we will talk about 2D crystal systems and lattices, but just before that a little bit more on point symmetries.

Under point symmetries, you have seen several of them, one was reflection, another was rotation, etc., but right now, since we are going to talk about two dimensions, these are the two important point symmetries that are present in the two-dimensional situation.

Now, why do we call them point symmetries and how are these point symmetries different from translation symmetry? Let me first define what a point symmetry is. After a point symmetry operation, there is at least one invariant point.

Now let us see what this definition means. Let us take a couple of examples to explain the meaning of an invariant point. Suppose I have a mirror, and on this mirror, I place an object on one side. This is what I will call an asymmetric object, since it has no symmetry, or we can say it has one-fold rotational symmetry.

This mirror will reflect the object onto the other side. If I call the first one a right-handed object, then after reflection, it becomes left-handed. Notice that all the points in space have moved after a mirror operation except for the points on the mirror itself. In the mirror line, no point moves, and such points are called invariant points. For a point symmetry, at least one invariant point should exist.

Now, consider the case of rotation. Suppose I have a three-fold rotational symmetry. The triangle symbol indicates that it is threefold. Consider an asymmetric object at some distance. Since it is threefold, we can rotate this axis by 120° . The object moves to another location and is copied there. Another 120° rotation brings the object to a new

position, and another 120° rotation brings it back to the starting point. In this rotation, there is no change in the handedness of the object.

The invariant points in this case are on the rotation axis. How does this differ from translation symmetry? In translation, every point moves in space, so there are no invariant points. Although the definition of invariant points may seem trivial, it becomes very useful when solving symmetry-related problems.

Now, let us look at 2D lattices in more detail. We want to examine the various crystal systems and the conventional unit cells used to define them. The same methodology can then be used to derive three-dimensional Bravais lattices. How do we do this? We add point symmetries to a translation vector.

Let the translation vector be \vec{a} , and the various point symmetries available are 1-fold, 2-fold, 3-fold, 4-fold, 6-fold, and in addition, a mirror. One by one, we will add these point symmetries to the vector \vec{a} and see the result of operating the point symmetry on the vector itself.

First, we consider 4-fold rotational symmetry. In an earlier lecture, we saw the square crystal system and the primitive square unit cell, which had 4-fold symmetry and several other symmetries. Let us take a look at that situation.

Let \vec{a} be the vector, and apply the 4-fold point symmetry on it. This vector rotates through 90° , which is one of the symmetry operations for 4-fold. We get another vector as a result of this operation; let us call this vector \vec{b} . Clearly, the angle $\alpha = 90^\circ$.

Based on this, we can get a unit cell and place the lattice points at the corners to obtain a primitive unit cell. Since there is a 4-fold symmetry, the unit cell naturally comes out to be square. Hence, the crystal system is called the square crystal system, and the unit cell defining the lattice has lattice points at the corners. In this case, $a = b$ and $\alpha = 90^\circ$.

Let us now consider a different unit cell to define the same square lattice. Drawing another adjacent square unit cell, again with lattice points at the corners, we get a new cell. Let us examine the lattice parameters. We can denote this as \bar{a}' and \bar{b}' , but \bar{b}' is equal to the original \bar{b} . The angle remains α .

One can quickly write that \bar{a}' is not equal to \bar{b}' , and $\alpha \neq 90^\circ$, but let us analyze this a bit. If you look at the \bar{a}' vector, it is a diagonal in the square unit cell. Since $a = b$ and $\bar{b}' = \bar{b}$, the ratio of the magnitudes of these two unit cell vectors, \bar{a}' over \bar{b}' , would be equal to the $\sqrt{2} \Rightarrow \frac{\bar{a}'}{\bar{b}'} = \sqrt{2}$.

It is straightforward to see that $\alpha = 135^\circ$, which is essentially $90^\circ + 45^\circ$. Even here, there are constraints on the lattice parameters or the unit cell parameters, and they are very specific. In the primitive square cell, these constraints result from the four-fold rotational symmetry. Hence, we should not directly judge the crystal system solely based on whether the parameters are equal or equal to 90° , as that can be misleading.

This makes it clear that the first unit cell developed based on a four-fold rotational symmetry is a square crystal system and the primitive square unit cell.

Now, let us add other symmetry elements. First, consider 1-fold symmetry, which means no symmetry. Starting with a vector a , since there is no symmetry, there are no restrictions on choosing the second vector \bar{b} , so it can be chosen arbitrarily. The shape of the unit cell is a parallelogram, with vectors \bar{a} and \bar{b} forming an angle α . This can be called a parallelogram crystal system, or more specifically, an oblique crystal system. Placing lattice points at the corners gives a primitive oblique lattice with no constraints on a , b , or α .

It is important to note that writing $a \neq b$ and $\alpha \neq 90^\circ$ does not mean equality cannot occur by coincidence. Experimental measurements, for example using X-ray diffraction, might show $a = b$ within experimental error. However, this does not automatically

determine the crystal system. The “not equal” notation can also be interpreted as “not necessarily equal” in some literature. The key point is that no constraints are assumed initially, and equality would indicate specific constraints.

Next, consider two-fold rotational symmetry. Take vector \bar{a} and apply a two-fold rotation, which is a 180° rotation. This flips vector \bar{a} in the opposite direction, but does not define vector \bar{b} . In a lattice, translation vectors work in both directions to generate the lattice, so this simply gives vector $-\bar{a}$. This means the second vector \bar{b} has no constraints relative to \bar{a} , and we again get a unit cell with angle α between \bar{a} and \bar{b} , and a not necessarily equal to \bar{b} . α can take any value. Thus, adding two-fold rotational symmetry still results in a primitive oblique lattice, the same as with one-fold symmetry. An oblique crystal can have either one-fold or two-fold symmetry.

We can say that the minimum requirement is one-fold symmetry; two-fold may or may not be present. So far, we have examined one-fold, two-fold, and four-fold symmetries. Now, we are left with three-fold, six-fold, and mirror symmetry.

Let us start with three-fold symmetry. Applying a three-fold rotational symmetry rotates vector \bar{a} by 120° and generates another vector \bar{b} . In this case, the magnitudes of the two vectors are equal. Placing lattice points at the corners gives a unit cell with $a = b$ and $\alpha = 120^\circ$ as one specific case.

Before naming this crystal system and the lattice, let us also consider six-fold symmetry. Applying a six-fold rotational symmetry involves a minimum rotation of 60° , though 120° rotation is also allowed. Performing a 60° rotation produces a possible unit cell in the shape of a rhombus with angles of 60° and 120° .

Now, six-fold symmetry means we can give a minimum rotation of 60° , though a 120° rotation is also allowed. Let us consider a 60° rotation. One possible unit cell that results is a rhombus with angles of 60° and 120° .

Comparing this unit cell with the one derived using three-fold symmetry, we see that they are not fundamentally different. Even in the three-fold case, the unit cell has a 60° angle. The difference is only in orientation, so both unit cells define essentially the same lattice. The symmetry could be three-fold or six-fold.

Both cases are grouped into a single crystal system, which we call the hexagonal crystal system. It is sometimes also referred to as trigonal, but we will use the name hexagonal. In this system, once the lattice points are placed and the unit cell is chosen, we have $a = b$ and $\alpha = 120^\circ$.

So far, we have developed three crystal systems: the square crystal system, the oblique crystal system, and the hexagonal crystal system.

We still have one point symmetry left to consider, which is mirror symmetry. We will see what happens when we add a mirror to a translation vector in the next lecture.

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Point Symmetries

- reflection, rotation, etc.
- after a point symmetry operation, there is at least one invariant point

(R) F (L) 7
m the mirror line no point moves

invariant points are on the 3-fold rotation axis

Translation Symmetry

- no invariant points

2D Lattices

- Crystal Systems
- Conventional Unit Cells
- Add point symmetries to a translation vector \vec{a} & \vec{b} 1, 2, 3, 4, 6-fold, m

4-fold

Square Crystal System
Primitive Square Unit Cell
 $a = b, \alpha = 90^\circ$ Constraints
 $\frac{a}{b} = 1, \alpha = 90^\circ$ Constraints

1-fold

Oblique Crystal System
Primitive Oblique
NO constraints on a, b and α

2-fold

Primitive Oblique (same as 1-fold)

3-fold

Hexagonal (Trigonal) Crystal System
 $a = b, \alpha = 120^\circ$

6-fold

So far 3 Crystal Systems