CRYSTAL SYMMETRY, X-RAY DIFFRACTION, AND PHYSICAL PROPERTIES

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Lecture 01: Lattice and Translation Symmetry

Welcome to the first lecture of the course, Crystal Symmetry, X-ray Diffraction, and Physical Properties. As the name implies, the course has three components. So, what are these three components? The first component is Crystal Symmetry, the second is X-ray Diffraction, and the third is Physical Properties.

This course focuses on these three components. The first component, Crystal Symmetry, is perhaps the most important one and will occupy more than fifty percent of the course. After completing this, we will move on to the remaining components. It is absolutely essential to study Crystal Symmetry first before proceeding to X-ray Diffraction and Physical Properties. Now, let us look at some of the salient features of these three components.

The salient features of Crystal Symmetry, for example, in a more general sense, are also referred to as Crystallography. Most students of Science and Engineering would have completed a basic course in Material Science, in which some part of Crystallography is included.

In this course, we will start from those basic components and move toward a much deeper understanding of Crystallography and Symmetry. In fact, symmetry is the basis of crystallography. Before I list the topics that I am going to cover today, let me first look at what we are going to study in X-ray Diffraction.

One of the topics we will look at in X-ray Diffraction is the Analysis of Crystal Structure. I will also introduce the concept called Reciprocal lattice and provide a brief overview of Experimental techniques.

In the Physical Properties part of the course, we will study properties such as Conductivity, Piezoelectricity, and Elasticity, among others. We will first look at their tensor representation and then understand the role of crystal symmetry in these properties.

Now, coming to Crystal Symmetry, in today's lecture, and in fact starting from today and continuing over the next two or three lectures, I want to introduce three key concepts: Lattice, Crystal, and Motif, which is also called basis. These three are the fundamental concepts to begin with.

There is often a lot of confusion regarding these terms, so it is important to first remove the misconceptions that usually arise from elementary courses in Material Science, where Crystallography is covered very briefly without going into its actual depth.

For instance, let us first consider the concept of a lattice. What is a lattice? A lattice is essentially an arrangement of points. To define it formally, a lattice can be described as a regularly spaced arrangement of points. These points can be considered in one dimension, two dimensions, or three dimensions.

Now, if we consider a crystal, it can be described as a regularly spaced arrangement of atoms. Similar to the lattice, this arrangement of atoms can exist in one dimension, two dimensions, or three dimensions.

If we examine these two definitions, the only difference is that in the case of a lattice, the arrangement is of points, whereas in the case of a crystal, the arrangement is of atoms. Because of the similarity in these definitions, a great deal of confusion and misconceptions can arise.

Some of these misconceptions will be encountered as we progress through this course, and my goal is to clarify and remove them. These misconceptions have often emerged because, in very basic Material Science courses, Crystallography is covered only briefly. In an effort to simplify the topic for easier understanding, certain concepts are sometimes presented incorrectly. In fact, even in several standard undergraduate textbooks on Materials Science, some of these incorrect notions are propagated.

My endeavor in this course will be to remove all misconceptions regarding Crystallography. Now, if we examine a lattice and a crystal, let us first consider their similarity. The similarity between the two is that both exhibit geometrical periodicity.

Now, let us focus on the differences. In the case of a lattice, it is an abstract geometrical entity, whereas in the case of a crystal, it is a physical entity.

Since a lattice is an abstract geometrical entity, it does not possess any physical properties. In contrast, a crystal exhibits physical properties. For example, a crystal may have Electrical Conductivity, may display Piezoelectricity, Elasticity, and may possess other properties such as Density, among others.

It is important to note this crucial difference: in one case, the lattice is an abstract entity, consisting only of a set of points in space, whereas in the second case, the crystal consists of atoms. The next question that arises is that, because these two concepts are so often confused, the terms lattice and crystal are sometimes used interchangeably, which leads to various confusions and misconceptions.

My job here is to make it very clear that a lattice and a crystal are distinct concepts. However, a natural question arises: what is the relationship between the lattice and the crystal? This leads us to the discussion of the relationship between a lattice and a crystal.

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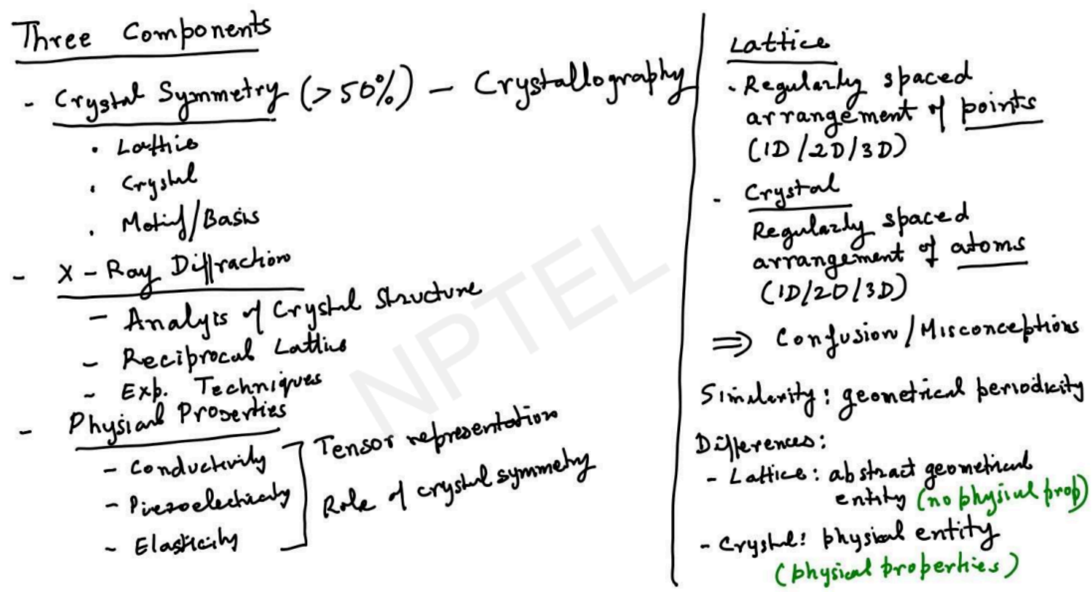

Let us now try to understand this. The important idea for establishing the relationship between a lattice and a crystal is the third key concept I introduced earlier, namely the motif or basis. Before we explore this relationship, it is necessary to first provide a clear definition of what a lattice is.

A lattice is sometimes also referred to as a point lattice. As mentioned earlier, it can exist in one, two, or three dimensions. Let us first consider an example in one dimension. Imagine a row of points that extends infinitely in both directions. The question then arises: what rules or conditions must these points obey?

This is a row of points. A lattice is a regularly spaced arrangement of points, which means that the spacing between consecutive points must be the same. The lattice can be defined by a vector, which we will denote as $\bar{a}$. This vector, also called a translation vector, connects one lattice point to the next lattice point.

Now, we can consider a vector defined as $n\bar{a}$, where n is an integer. This means that n can take values from minus infinity to plus infinity, such as -3, -2, -1, 0, 1, 2, 3, and so on.

Here, the lattice extends to plus infinity in one direction and minus infinity in the other. The vector $n\overline{a}$ is also referred to as a lattice translation vector.

This is a lattice translation vector, which we can denote as $\overline{r}$, where

$$\overline{r} = n\overline{a}$$

This means that by choosing different values of n, we can reach every lattice point. In other words, the entire one-dimensional lattice can be generated by varying n.

Another definition of a lattice, often found in textbooks, states that each lattice point has an identical environment in the same direction. In the one-dimensional case, of course, this direction is unique. However, in two or three dimensions, there are infinitely many directions to consider. In any direction you choose to travel from one lattice point to another, the lattice points should appear equally spaced.

Let us now consider an example in two dimensions. A two-dimensional lattice can be represented as a small portion of an infinite lattice extending in all directions. Imagine that these points are arranged along two perpendicular directions: the x-direction and the y-direction. Along the x-direction, the lattice extends from minus infinity to plus infinity, and similarly, along the y-direction, it also extends from minus infinity to plus infinity. Thus, this forms an infinite two-dimensional lattice.

Now, let us consider the translation vectors in two dimensions. We can denote one vector as $\overline{a}$ and the second vector as $\overline{b}$. The lattice translation vector, denoted as $\overline{r}$, can then be expressed in terms of two integers as:

$$\overline{r} = n_1\overline{a} + n_2\overline{b}$$

where n_1 and n_2 are integers.

This lattice translation vector allows us to start from any lattice point and reach any other lattice point. In other words, the lattice translation vector can be used to generate the entire infinite lattice.

I always keep saying that the lattice is considered infinite because, according to its very definition, each lattice point has an identical environment in the same direction.

For example, if I have to travel from here to here, I get some spacing. The spacing in this case will be $\overline{b}$, again $\overline{b}$, and so on, the same spacing. If I want to move from this lattice point to this lattice point, this will be a different spacing, and from the second to the third, it will be the same spacing as before.

Here, if it is $\overline{b}$, then in this direction it will be some spacing $\overline{r}$, which will be a function of both $\overline{a}$ and $\overline{b}$. One can even consider a direction like this; again, we will get equally spaced lattice points, but with a different spacing. This definition illustrates what is meant by an identical environment in the same direction.

Another point is that we keep saying it is an infinite lattice. We say this because the very definition of the environment being identical implies that, if it were a finite lattice, for example, if I consider this point where I have reached a boundary, then this point would not have the same environment.

If I want to travel in this direction, I do not see any lattice points here. Therefore, the very definition of an identical environment in the same direction implies that the lattice must necessarily be infinite. I hope this makes it clear what a lattice of points is.

One important point is the defining property of a lattice. The defining property of a lattice is, in fact, a symmetry, which is called translation symmetry. If an arrangement of points does not have this translation symmetry, then it cannot be called a lattice from a crystallographic point of view. I think it will be useful to consider an example of an orderly arrangement of points that is not a lattice.

Let us consider that. To draw the lattice points, I am first drawing regular hexagons, similar to a honeycomb structure. You can imagine that this forms a space-filling arrangement extending to infinity. I then place lattice points at the corners of these hexagons. Thus, we have a perfectly regular arrangement of points, but this arrangement is not a lattice.

Now, why do I say this? We go back to the definition of a lattice: identical environment in the same direction. Let us identify a few lattice points. I will denote one lattice point as A and another as B. Now, consider the translation from lattice point B in this direction. Let us denote this translation vector as A in a given direction, and we move from B to another lattice point, C.

Now, consider the same translation from lattice point A. In this case, the translation does not end at a lattice point, which means that the environment of points in the same direction at B and A is different. This is the reason why this arrangement cannot be called a lattice.

I hope this definition of a lattice is now clear. At this point, the next topic we will consider is a crystal and how a crystal is related to the lattice and motif. The discussion of these relationships will be the subject of the next lecture.

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