

Solid State Physics

Lecture 1

What is solid?

Hello all. Welcome to the course on condensed matter physics. Here we will start our discussion with the structure of solids. In order to discuss the structure of solids, we must discuss the crystal structure first. (Refer Slide Time: 00:44)

Solid is a periodic array of atoms and in this periodic array of atom we can have different structures, different kind of periodic arrays are possible. And X-ray was the first tool, using diffraction of X-ray, we could find the structure of solid; we could determine it from experiments. So, to begin with we must define a crystal. How do we define a crystal?

A crystal is composed of a lattice, which is a mathematical concept plus a basis. Now, basis is a group of atoms; this is not the kind of basis that you know in the context of vector space, it is just a group of atoms. So, how do we define lattice? An ideal crystal is constructed by infinite repetition of identical group of atoms, such a group is called basis and this basis is attached to a set of points and that set of points is called lattice, together they generate a crystal.

The lattice in three dimensional space, may be defined as three translation vectors; \vec{a}_1 , \vec{a}_2 and \vec{a}_3 , these three translation vectors. Now, we will see how these translation vectors define a crystal, well define a lattice. The idea of these translation vectors is similar to that of the basis vectors that you have learnt in the context of vector space; but these are not called basis here, basis in this context is just a group of atoms and we will come to that discussion later.

So, let us consider a situation where there are three vectors in a three dimensional space. This is \vec{a}_1 , say a vector like this is \vec{a}_2 , and another vector like this is \vec{a}_3 . Although I have drawn all these three vectors on a plane, these are not coplanar; these well of course two vectors will make a plane, but the third vector is outside the plane. And that will make a parallelopiped in a three dimensional space and that parallelopiped is called the cell or the unit cell of the system.

So, the arrangement of atoms at a at a position say \vec{r} vector that would be same as the arrangement of atoms somewhere else, because we have infinitely periodic arrangement of atoms. So, if we have \vec{r}' prime that would be \vec{r} ; that is any point that is the coordinate of any lattice point plus some linear combination of the lattice vectors $u_1\vec{a}_1 + u_2\vec{a}_2 + u_3\vec{a}_3$ like this, where u_1 , u_2 , u_3 these are arbitrary integers.

If these are integers if \vec{r} represents a lattice point, then \vec{r}' will represent a similar kind of a lattice point after this addition of this linear combination of the primitive the lattice vectors, ok. So, let us now define what is primitive lattice? So, primitive lattice is the smallest possible volume of a cell that comprises a lattice; that makes a lattice that is the building block of the lattice. So, there is no cell that is of smaller volume. So, what is the volume in this context?

The volume would be given as the scalar triple product of these lattice vectors. In case of primitive lattice, this volume would be the minimum and this can serve as the building block for describing the crystal structure, the entire crystal structure. The associated translation vectors are primitive translation vectors.

So, in this context, if this triple product gives us the minimum volume of the building block for describing the crystal; then \vec{a}_1 , \vec{a}_2 and \vec{a}_3 these are the primitive translation vectors.

Non-primitive translation vectors are often used; that means those would be bigger than these translation vectors and may point along some other direction. They are often used if that helps understand

the symmetry of the system in a better way. Otherwise primitive lattice is fine, we can use primitive lattice. (Refer Slide Time: 07:15)

Now, let us go to the discussion of basis in and the idea of crystal structure. As we said earlier, the basis of the crystal structure can be identified once the crystal axis, that is the lattice vectors are chosen and it is a group of atoms.

So, if we have say lattice points somewhat like this and we describe the lattice vectors like this; I am drawing it in two dimension for simplicity. I have a two dimensional screen, so it is easier to represent it accurately in two dimension. If I do this, if I choose the lattice vectors this way; then we have lattice points represented by the small circles and lattice vectors represented by the arrow heads \vec{a}_1 and \vec{a}_2 .

Now, each lattice point there would be an attached basis system, that means a group of atom. Whatever that group may look like, but when you attach that group of atoms to every such lattice point, you will get a crystal and it has to be infinitely repeated in ideal sense.

Of course there is nothing called infinity; but when the number of repetitions is of the order of Avogadro number, we call it infinitely repeated. So, the number of atoms in a basis may be one or more than one; the position of an atom j for example, of the basis relative to its lattice point can be given as \vec{r}_j that equals $x_j\vec{a}_1 + y_j\vec{a}_2 + z_j\vec{a}_3$. So, making the associated lattice point; the origin we can have the values for x_j , y_j and z_j ranging between 0 and 1. So, we are setting the origin at the lattice point. So, the basis atoms will have this kind of position vector and x_j , y_j and z_j that is the coefficients of these lattice vectors that will range within 0 and 1, it may be fractional.

So, what is the primitive unit cell? The parallelepiped defined by the primitive axis \vec{a}_1 , \vec{a}_2 and \vec{a}_3 that is called the primitive unit cell. A primitive cell is the minimum volume cell that we have said earlier; there are many ways of choosing the primitive axis and the primitive cell for a given lattice.

But the number of atoms for a primitive lattice or primitive basis is always the same for a given crystal structure. There is always one lattice point per primitive cell; I did not mean one atom, just one lattice point. With that lattice point, there may be multiple atoms attached.