

# Solid State Physics

## Lecture 2

### Bravais Lattice

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So, now, let us discuss different fundamental types of lattices. Crystal lattices can be mapped into themselves by various symmetry operations and that makes different fundamental types of lattices; the first kind of symmetry operation that is a must for every crystal is translation. (Refer Slide Time: 01:15)

So, if we translate one atom, one lattice point to using this kind of a relationship, translation of  $u_1\vec{a}_1 + u_2\vec{a}_2 + u_3\vec{a}_3$ , where  $u_1$ ,  $u_2$  and  $u_3$  are integers; this will find a similar kind of point. So, this kind of translation would map the crystal itself, mapped to the crystal itself. So, we will have every solid structure that is symmetric to this kind of that is invariant to this kind of an operation that is translation. There are other symmetry operations often in a lattice; rotation about an axis that passes through a lattice point, that could be an operation. So, in lattices, we can find 1 fold, 2 fold, 3 fold, 4 fold or 6 fold rotation operators, operations possible, that maps the crystal to itself. So, the associated rotation angles are for 1 fold it is  $2\pi$ , for 2 fold it is  $\frac{2\pi}{2}$  that is pi, for 3 fold  $\frac{2\pi}{3}$ , 4 fold is  $\frac{2\pi}{4}$  that is  $\frac{\pi}{2}$  and for 6 fold it is  $\frac{2\pi}{6}$ , that is nothing but  $\frac{\pi}{3}$ . We cannot find a lattice that goes into itself under other rotations. If we have  $\frac{2\pi}{7}$  or  $\frac{2\pi}{5}$ , these kind of rotation angles we would not map the lattice to itself in that kind of an operation. While it is possible for a molecule to have any degree of rotational symmetry and you are familiar with it; an infinite periodic lattice cannot have that. So, try this disproving this statement by drawing pictures, imagining it yourself, looking at the computer screen whatever way you like and you will appreciate this statement better, ok. (Refer Slide Time: 03:51)

Now, let us move onto different lattice systems in 2 dimension. This is for simplicity; our world is 3 dimensional, so we will have to learn about 3 dimensional lattices. So, there are 5 different types of lattice in 2 dimension, these are called Bravais lattices. The first one is there is no symmetry there. So, in 2 dimensional case, we will have 2 lattice vectors a 1 and a 2. So,  $\vec{a}_1$  and  $\vec{a}_2$  are not equal and the angle between them is also arbitrary, that is the least symmetric situation. And there are special lattices; that means more symmetric situation than the first one, those could be square lattice for example. How do we have a square lattice? We will find a square like this; does not really look like a square, so maybe I modify the picture a bit, I draw this up to here and that gives me a square. The corners are lattice points and this vector is say  $\vec{a}_1$ , this vector is  $\vec{a}_2$ , and the angle between them is  $\phi$ . So, in the case of a square lattice, we have the magnitude of  $\vec{a}_1$  equals the magnitude of  $\vec{a}_2$  obviously, and the  $\phi$  angle is  $90^\circ$ , that defines a square lattice. We can have hexagonal lattice in 2 dimension. How would a hexagonal lattice look? An atom at the center of the hexagon; then sorry a lattice site at the center of the hexagon, not atom. And similarly one here, one here, one here, one here; repetition of this will make a hexagonal lattice, we can have lattice vectors like this and this. And this will give us, as you can see from this picture  $\vec{a}_1$  equals  $\vec{a}_2$  and this angle here  $\phi$ ; for a regular hexagon, this angle would be  $120^\circ$ . We can also represent hexagonal lattice like this, say we have  $\vec{a}_1$  drawn like this,  $\vec{a}_2$  drawn like; this is not a different picture although the angle is different, its exactly similar kind of a representation. And we can have rectangular lattice certainly. As the name suggests, we will have  $\vec{a}_1 \neq \vec{a}_2$  and the angle  $\phi$  would be  $90^\circ$ . If we draw it, we will have something like this with the lattice points at the corners. This is  $\vec{a}_1$ , this is  $\vec{a}_2$  and this thing repeated; that will give us a rectangular lattice. (Refer Slide Time: 08:30)

We can also have centered rectangular lattice. Centered rectangular lattice is something like this; say we have a lattice site here, one lattice site here, one here, one here and one here, we draw one vector  $\vec{a}_1$  like this, another lattice vector  $\vec{a}_2$  like this. Here this is a centered hexagonal, sorry centered

rectangular lattice, where at the center of the rectangle there is one lattice site. So, this you can clearly see is not a primitive lattice; because there are more than one lattice sites in the unit cell that we have considered. So, its not a primitive unit cell. How about we move onto three dimensional lattice types; let us see how it goes there. We can have 14 different lattice types in three dimension, these are called Bravais lattices. Out of these 14, one is the least symmetric one and 13 special lattice types. Let us tabulate these things. So, we will write it, we will make a table like this the system; then we will put the number of such lattices, then its attributes. If we try to classify lattices in this way, then the first thing that comes is triclinic; that is the least symmetric one and there is only 1 type of lattice. Its attributes are because its the least symmetric one,  $\vec{a}_1 \neq \vec{a}_2 \neq \vec{a}_3$  and the angles between these lattice vectors  $\alpha$ ,  $\beta$  and  $\gamma$ ; they are all different, alpha not equals beta not equals gamma. Then a little bit higher symmetry is monoclinic, 2 such lattices are possible and its attributes are all the lattice vectors are of different length,  $\vec{a}_1 \neq \vec{a}_2 \neq \vec{a}_3$ ; but we have  $\alpha = \gamma = 90^\circ$ , while  $\beta \neq 90^\circ$ . The next one is orthorhombic, there can be 4 different types of orthorhombic lattices; here we have  $\vec{a}_1 \neq \vec{a}_2 \neq \vec{a}_3$ , but all the angles are  $90^\circ$ . Then comes tetragonal; in tetragonal we can have 2 lattice types and its attributes are  $\vec{a}_1 = \vec{a}_2$  but that is  $\neq \vec{a}_3$  and the angles are  $90^\circ$ . So, we are moving higher up in the symmetry ladder, then comes the cubic. Cubic has 3 variants; we will discuss all 3 variants of cubic, although we would not discuss the variants of other lattice types. You can find it out over internet if you are curious or; because those are more clumsy, we will avoid discussing that here. For cubic it is obvious that  $\vec{a}_1 = \vec{a}_2 = \vec{a}_3$  and all the angles are  $90^\circ$  indeed. After cubic we go to trigonal, there is only one type and here the attributes are  $\vec{a}_1 = \vec{a}_2 = \vec{a}_3$  and the angles  $\alpha = \beta = \gamma$ ; but none of the angles are  $90^\circ$ , it is  $< 120^\circ$ ,  $\neq 90^\circ$ . And the last one is hexagonal, only one type of hexagonal is possible; here  $\vec{a}_1 = \vec{a}_2$ ,  $\vec{a}_3$  is different,  $\alpha$  and  $\beta$  are  $90^\circ$ ,  $\gamma = 120^\circ$ . So, here we have defined different Bravais lattices for three dimensional structure. After defining this, let us see a few examples; more specifically we want to see the three examples of cubic lattice structures that will be very instructive. (Refer Slide Time: 15:53)

So, the first kind of cubic lattice is called simple cubic. As the name suggests it is really simple, you have to draw just a cube like this. And at each corner there is a lattice site, this is the simple cubic structure. So, can you find out how many lattice points are inside the cell in this cubic cell? So, you can see that, if we have a sphere at each corner, only one eighth of that sphere would be inside this cube; that means there are 8 corners and each corner has one eighth of a lattice site. So, in total there is only 1 lattice site inside this cube. And how many nearest neighbors do we have, ok? If we count the nearest neighbors here; we can see, we can take this lattice site for example, and we can see that its 1, 2, 3 equidistant points and similarly we can extrapolate to one below, one behind and one at the left. So, there would be 6 nearest neighbors of this lattice site, ok. And the lattice vector for simple cubic; the set of lattice vectors is very simple. You can just write  $\vec{a}_1 = a$ , that is the lattice constant along the  $\hat{x}$  direction;  $\vec{a}_2$  that is  $a\hat{y}$ , and  $\vec{a}_3 = a\hat{z}$ , it is so simple, these are the lattice vectors. Now, let us move onto body centered cubic, its called bcc, ok. How do we draw a body centered cubic structure? Let us try something similar; let us first draw a cube and of course at each corner, we will have a lattice site just like the simple cubic one. What is additional here? As the name suggests, at the center of the body we will have a lattice site. Let us try to draw it a bit better, maybe it will come somewhere here; at the center of this cube we will have a lattice site, that makes it a body centered cubic structure. So, now you are supposed to find how many lattice points are inside the cell and its your homework and also count the nearest neighbors, ok. Now, let us consider the lattice vectors. The lattice vectors, well you can clearly see that this bcc is not a primitive cell; if we talk about. So, this kind of a cell bcc which is symmetrically cubic, but the primitive cell is something different that has a lower symmetry; we can represent it as a cube and then the lattice vectors would be exactly similar like the simple cubic one. But if we want to find the primitive lattice vectors of this, then the primitive lattice vectors would be different from that of simple cubic. The primitive lattice vectors in this context would be, sorry it is  $\frac{1}{2}a$ ,  $a$  is the lattice constant and  $\vec{a}_3 = \frac{1}{2}a(\hat{x} + \hat{y} - \hat{z})$ . These are the primitive lattice vectors in case of bcc structure and your work is to verify this; by repeating this

unit cell, drawing a picture, imagining it, whichever way you want, ok. After discussing the primitive unit cell for bcc, let us move onto the face centered cubic structure, its called fcc. (Refer Slide Time: 23:14)

Let us first draw a structure; obviously the corner makes lattice points. And as the name suggests, we will have other lattice points at the centers of the faces; bottom face, top face, side faces, and front and rear face, all these are lattice sites. When we have this kind of a structure; now again the similar to earlier, your homework is to find the number of lattice points inside the, inside this unit cell and also find the number of nearest neighbors. After finding this, I am giving you the, you need the lattice vectors corresponding to the primitive unit cell in this context, you need to verify that. For the primitive unit cell, that is the primitive lattice vectors; we can write here in case of fcc,  $\vec{a}_1$  is given as  $\frac{1}{2}a(\hat{x} + \hat{y})$ ,  $\vec{a}_2$  is given as  $\frac{1}{2}a(\hat{y} + \hat{z})$ , and  $\vec{a}_3$  is given as  $\frac{1}{2}a(\hat{z} + \hat{x})$ . So, you can see that fcc is also not a primitive unit cell; the primitive unit cell is smaller than this conventional cubic cell. Now, I ask you to perform another task, that is find out the volume of the unit cell, the primitive unit cell for bcc and for fcc; this is also another homework. You know how to find the volume of a cell; it is just a triple product, scalar triple product  $\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)$ , that will give you the triple product, that will give you the cell volume. And you need to find the cell volume and compare with the simple cubic one that is the task. So, here we have discussed about different Bravais lattices and we have carefully analyzed the cubic lattices. There are three possible cubic lattices; one is simple cubic, that is as the name suggests it is pretty simple, body centered cubic and face centered cubic. We have learned its structure and you need to work out some of these problems that we have discussed to understand the, to generate a feeling of yourself about the crystal structure.