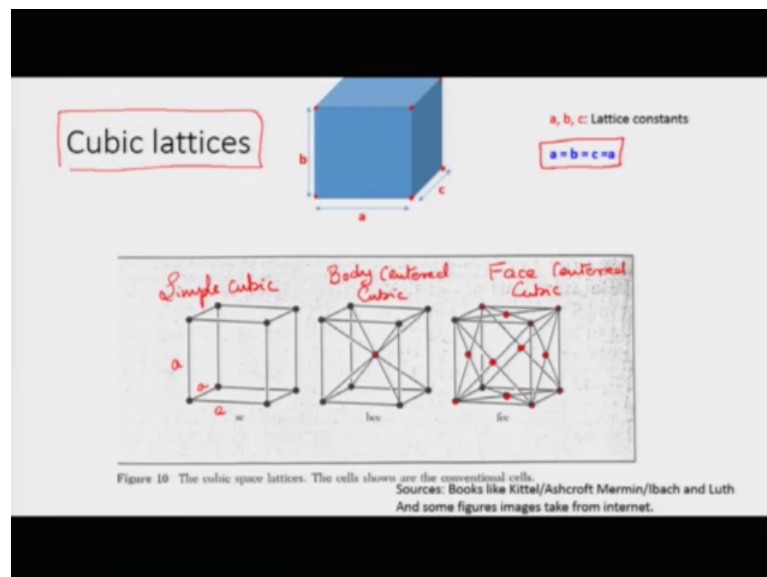


Introduction to Solid State Physics
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Lecture - 31
Introduction to different crystal type Part-I

In the last lecture, we came across with the concept that you have many different types of Bravais lattice which are just the set of points, a geometrical set of points with some properties which I have already told you about, what classify points as a set of points belonging to a Bravais lattice. However, another important property of these points is that if they obey that they remain invariant this lattice this collection and arrangement of points if it remains invariant under some particular symmetry operations. Like one of the rotations or one or more of the mirror operations or one or more of the inversion operations if the system remains invariant under these operations, then you get special class of Bravais lattices, which are important and those Bravais lattices are studied separately.

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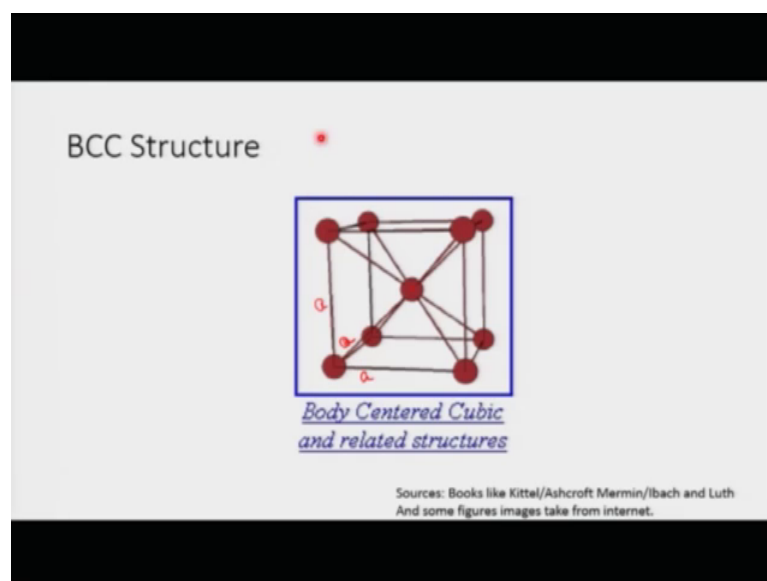
And amongst those 14 set of Bravais lattice is an important set which is falls amongst the cubic lattices. And as the name suggests the points are arranged at the corners of the cube. The spacing between consecutive lattice points is your lattice constant. And for a

cubic system the lattice constants are exactly identical you know for a cube the sides of the cube have the same length. So, it is natural that the name comes as cubic lattice. So, this is the simple cubic lattice, lattice, where the points are arranged at the corners of the cube, and a is equal to, a is the same along all the different directions the lattice constants are identical

A variant of this simple cubic structure is the body centered cubic structure, the body centered cubic structure, where the lattice points are organised at the edges of the cube, but there is one extra point which is sitting at the centre of the cube. This also follows some symmetry operations remains invariant under certain symmetry operations. And this is called as a body centered cubic structure.

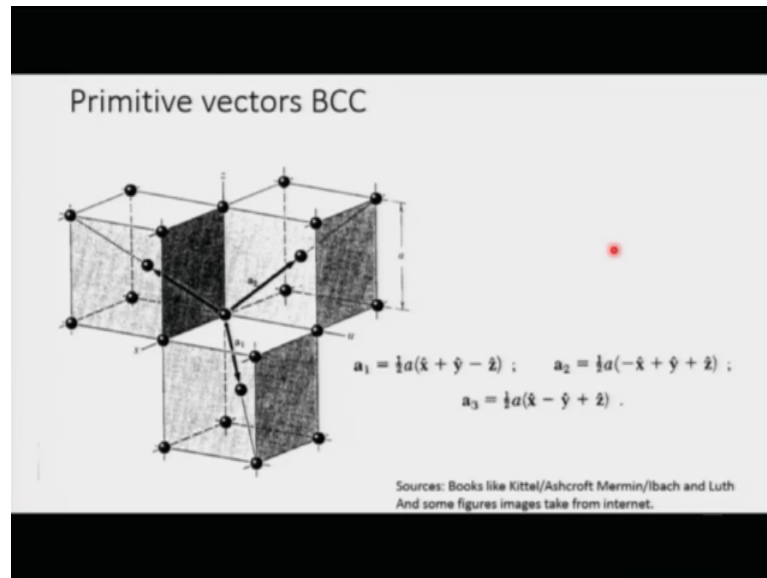
And finally, within this class of cubic lattices, we have the face centered cubic structure, where again you have points which are at the edges of the cube, you have points which are sitting at the edges of the cube. But additionally on each of the cube faces you have points which are sitting at each of the cube faces the top and bottom face, the side faces, the four side faces have points which are sitting at the centre of each of these faces. So, you have the simple cubic, you have the body centered and the face centered cubic structure. The simple cubic is obviously, the simplest of the structures and it is very easy to analyse these structures. Amongst the other structures we will now look at these crystal lattices in a little bit more detail.

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So, first we look at the body centered structure. The body centered structure as I said has atom at the corners of the cube and has a atom at the centre. And the lattice parameters are a and a , the lattice parameters are exactly identical. So, you have atoms which are sitting on the corners of the cube, and one in the body of the cube which is in the centre of the cube and this is your body centered cubic structure.

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Now, for this body centered cubic lattice of atoms, you can actually translate this entire structure over the entire space, this collection of lattice points you can translate it over the entire space, this set of points you can move it along the x , you can move repeat the same thing along the y , z , minus x , minus y , minus z direction. And you will fill up the entire space ok. So, you have here body centered cubic structure lattice.

And then you can try and define what are the fundamentals or what are the primitive lattice vectors in this lattice. So, the primitive lattice vectors in this lattice this is BCC lattice this is indicating one BCC structure another BCC structure another BCC structure, there will be one in between, and then they will go in all three directions.

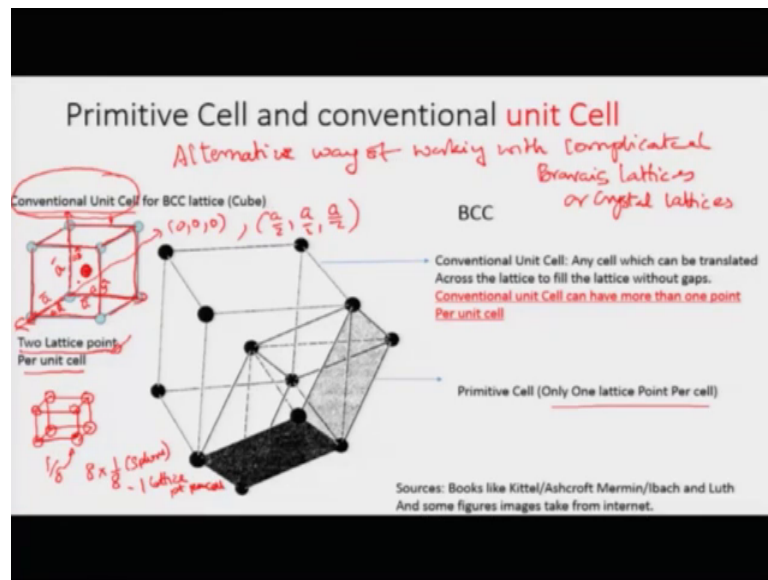
Now, if you want to define the fundamental one of the ways of defining the primitive vector which will have only one lattice per point, it will define and of course, first an area in which you will have only one lattice point per cell per primitive lattice cell. And the corners of it or the it will defined by the primitive lattice vectors, then one way of

showing the primitive lattice vectors, one choice of primitive lattice vectors for the BCC is this.

If these are the three cardinal directions the x, y and z direction, the x-direction shown here, the y which is along this direction and the z along this direction which are the along the corners of a cube. But these directions do not form your primitive vector directions rather the primitive vector directions are the primitive lattice vectors are one which is along this, one which is along this and one which is along this. So, from one corner of a cube the vectors are pointing towards a BCC point towards a body centered point which is sitting in all the adjoining crystals or in the adjoining lattices. The adjoining BCC lattice it is pointing towards the adjoining BCC points.

So, in terms of x, y and z you can write your a 1 as half of a x cap plus y cap minus z cap ok. It is in the x y plane plus x and plus y cap directions and this is in the minus z cap direction. Similarly, a 2 will be in the minus x cap direction and this will be in the minus y cap directions. So, these are your primitive vectors for the BCC lattice.

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And if those are the primitive vectors, this is your primitive cell ok. If you look at your BCC lattice, you can define your primitive cell which is the smallest volume of lattice points which will have only one lattice point per cell a 1, a 2, a 3 which are the primitive lattice vectors I have already shown you. And this is the volume which is made by the primitive lattice vectors, the primitive lattice volume and it is pretty complicated. So, as

the lattices get more and more complicated, your primitive lattice cells can also get more and more complicated. Of course, there is no it is not a unique choice, this is one way you can also draw the Wigner Seitz cell for this which I leave it to you to look up in a book like Ashcroft and Mermin where the Wigner Seitz cell for a BCC lattice is already shown in the book. So, you can go and take a look at it and you will see it is a pretty complicated three-dimensional structure.

So, the primitive cells actually become more and more complicated as the nature of the crystal structure becomes more and more complicated. BCC is one example where you can draw it and show it that this is your primitive cell. However, an alternative way of defining such sort of lattices is using another way. So, you have an alternative way of working with complicated Bravais lattices or crystal lattices in general. So, BCC is one sort of a slightly complicated lattice where you have one point in the centre of the cube, and its primitive cell is a little complex complicated.

But is there another way to analyse the structure? So, instead of drawing a primitive cell you can actually consider the BCC as having a conventional unit cell. And what is the conventional unit cell, the conventional unit cell is any cell which can be translated across the lattice to fill it up without gaps. So, I can instead of having this sort of a lattice primitive cell which I have shown here ok, instead of this primitive cell and translating it across to fill up the entire lattice, I can also consider that the BCC unit cell is a conventional unit cell which is a cube, it is just this cube and I can fill up the entire space with the cube.

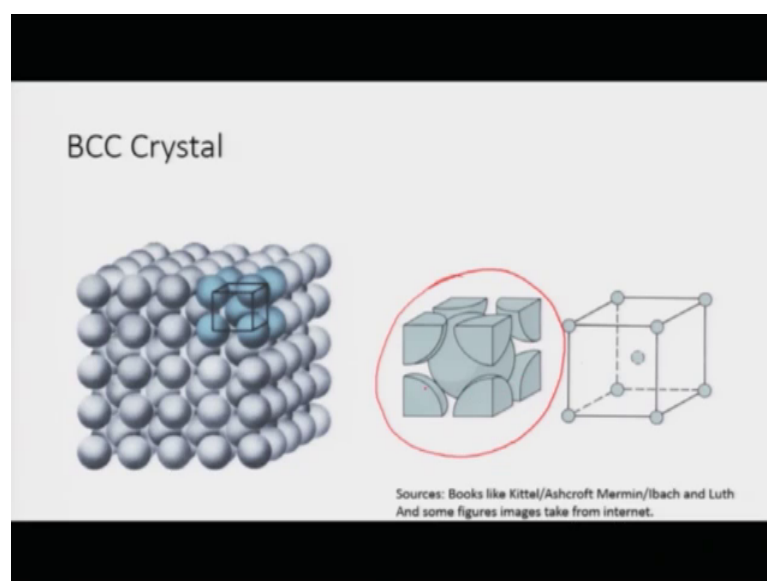
The only requirement is now that associated with this cube is there will be two lattice points per unit cell, because a cube as I had told you earlier has only one lattice point per cell. Recall that if you consider a cube, if you consider this cube and if you have spheres at the corners of the cube only one-eighth of each is belonging to this cube and there are eight such points. So, eight into one-eighth of a sphere will give you one lattice point per cell, where for a conventional cube, but a body centered has another point which is sitting in the centre. You have this additional point which is sitting in the centre, so one point per cell comes from the corners of the cube and another point comes from the body centered point.

So, instead of describing the body centered lattice with the complicated primitive cell, we define it with using a conventional cubic cell, but with two lattice points per cell. A primitive lattice has only one lattice point per cell; a conventional unit cell can have more than one point per cell, but it makes description of these lattices a little easier. So, you can describe a BCC not with this primitive cell, but you can describe it with a cubic unit cell.

And you can define your primitive vectors along these three directions with the only requirement that there are two points per conventional cell. So, your conventional cell, these are the vectors \hat{a} , \hat{b} , \hat{c} , these are your fundamental translation vectors. And you can define the location of the two points per cell one is that $0, 0, 0$ and the other is at $a/2, a/2, a/2$. This is the location of the two points per conventional unit cell. And if you translate this now across the entire cell, you will make up the entire lattice.

And this is an important point that often we do not always go back to a primitive cell wherever required we do it, but sometimes we also describe a complex lattice structure with its conventional unit cell which can be a simple structure like a cube and associated with it are more than one lattice points. So, this is as far as BCC structure is concerned ok.

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And here actually it shows you very nicely that why there are two points per cell, the big circle in the centre or the big sphere in the centre is your lattice point. And the one-eighth of each sphere is sitting at the corners of the cube.

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Elements with BCC Structure

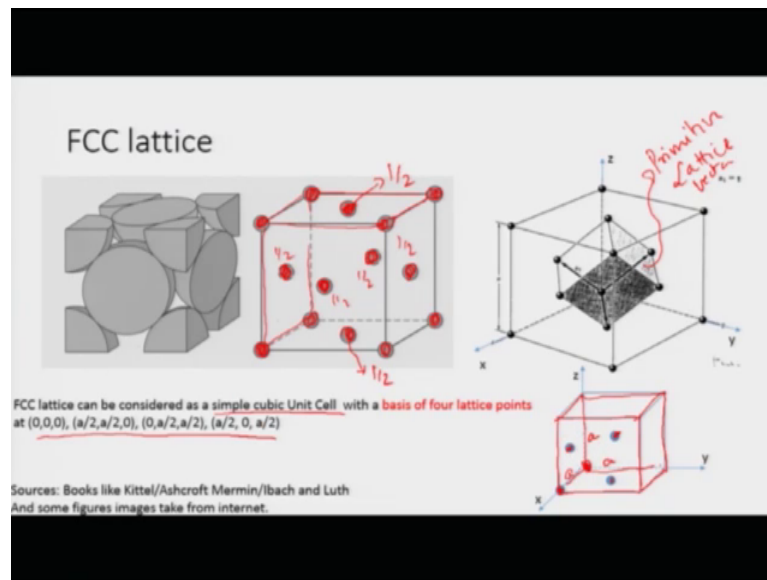
Table 4.2
ELEMENTS WITH THE MONATOMIC BODY-CENTERED
CUBIC CRYSTAL STRUCTURE

ELEMENT	a (Å)	ELEMENT	a (Å)	ELEMENT	a (Å)
Ba	5.02	Li	3.49 (78 K)	Ta	3.31
Cr	2.88	Mo	3.15	Ti	3.88
Cs	6.05 (78 K)	Nr	4.23 (5 K)	V	3.02
Fe	2.87	Nb	3.30	W	3.16
K	5.23 (5 K)	Rb	5.59 (5 K)		

Sources: Books like Kittel/Ashcroft Mermin/Ibach and Luth
And some figures images take from internet.

Elements which form BCC structure there are a large variety of elements which I have enlisted here ok. And this is the lattice parameters. This is the lattice constants or the lattice parameters of those structures. And for example, barium, potassium, sodium rubidium and these are few examples where you can see they form a BCC structure. So, large number of elements form a BCC structure.

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Next we go to the FCC lattice - a face centered lattice. A face centered lattice is as I had said that you have a on the faces of each cube, you have a lattice point along with points which are sitting at the corners of the cube. So, you have points which are sitting on the faces of each edge of a cube as well as on the corners of the cube. So, this is your face centered cubic structure.

For the face centered cubic structure, you can define your primitive lattice vectors as shown here. Apart from that you can define it also using what I told you earlier that the face centered cubic structure can be defined using a simple cubic unit cell. This is your conventional unit cell, also called as a unit cell, this is not the primitive unit cell this is your conventional unit cell which is a simple cube which is drawn here. But now instead of one lattice point per cell, the conventional unit cell for the face centered cubic structure has four lattice points per cell. One lattice point comes from the cube of points which are sitting at the corners of the cube, and the remaining three come from the edges.

For example, half of this belongs to this face; similarly half of this belongs to this face. So, these two halves makeup one lattice point; similarly half from here, half from here, and half from here, half from here. So, you will get three from the 6 faces 3 lattice points from the 6 faces, and one lattice point which is associated with the corner of the cube. So, the FCC structure can be considered or described with a simple cubic unit cell with

lattice parameters a , and these are the fundamental vectors. These are not the primitive vectors these are the fundamental vectors. Primitive vectors are shown here ok, but this conventional unit cell has four lattice points per cell. One is sitting at the origin, and the three are at a by 2 , a by 2 , 0 , 0 , a by 2 , a by 2 , a by 2 , 0 , a by 2 . So, these are the three four lattice points for the FCC structure.

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Elements That Have FCC Structure

Table 4.1
ELEMENTS WITH THE MONATOMIC FACE-CENTERED
CUBIC CRYSTAL STRUCTURE

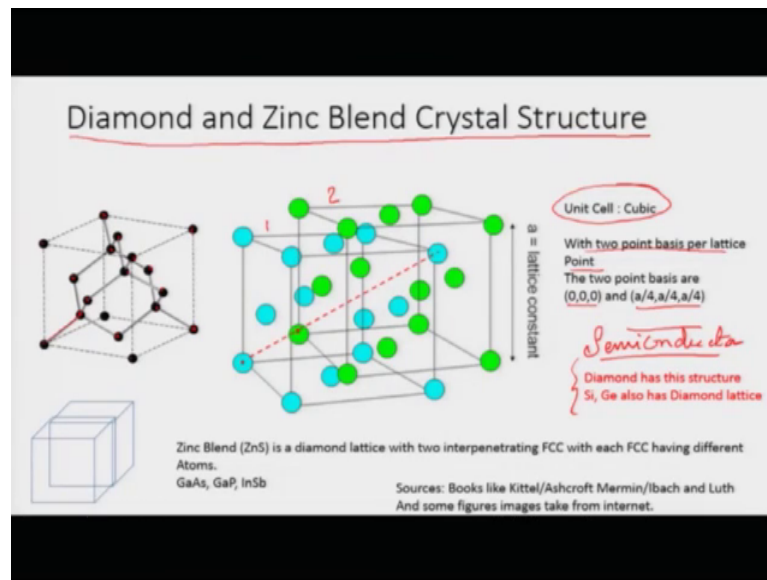
ELEMENT	a (Å)	ELEMENT	a (Å)	ELEMENT	a (Å)
Ar	5.26 (4.2 K)	Ir	3.84	Pt	3.92
Ag	4.09	Kr	5.72 (58 K)	β -Pb	4.64
Al	4.05	La	5.30	Rh	3.80
Au	4.08	Ne	4.43 (4.2 K)	Se	4.54
Ca	5.58	Ni	3.52	Sr	6.08
Ce	5.16	Pb	4.95	Tl	5.08
β -Co	3.55	Pd	3.89	Xe (58 K)	6.20
Cu	3.61	Pt	5.16	Yb	5.49

Data in Tables 4.1 to 4.7 are from R. W. G. Wyckoff, *Crystal Structures*, 2nd ed., Interscience, New York, 1963. In most cases, the data are taken at about room temperature and normal atmospheric pressure. For elements that exist in many forms the stable room temperature form (or forms) is given. For more detailed information, more precise lattice constants, and references, the Wyckoff work should be consulted.

Sources: Books like Kittel/Ashcroft Mermin/Ibach and Luth
And some figures images take from internet.

For the FCC structure, again one can define one knows that there are various elements which can actually form the FCC structure, a large variety of elements can form the FCC structure. For example, the argon gas can actually form a solid at very low temperatures, and this solid is actually an FCC structure. Aluminium is an FCC lattice ok and similarly lanthanum and so on ok. So, all these different types of elements form a face centered cubic crystalline solid. So, this is another type of crystalline lattice that one encounters.

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Next we come to a slightly more complicated lattice, and these two lattices are related to each other the diamond and the zinc blend crystal structure. Diamond you already know is made up of carbon atoms and the carbon atoms form a solid in diamond they form a solid crystal structure. And this is the position of the atoms in a diamond lattice, and you see it is pretty complicated ok. The atoms are located not only at the corners of a cube, but there is a complex distribution of these atoms inside the cube.

One way to think about this diamond lattice which is these points which are arranged at these locations all these points this is definitely not a Bravais lattice. The diamond lattice is not a Bravais lattice, but this lattice can actually be described quite nicely by if I consider one FCC lattice, suppose this is an FCC lattice where I have points on the corners of the cube. And if it displace this lattice suppose I have two FCC lattices which I displace from one from each other and move the second lattice with respect to the first along the body diagonal ok. If I displace the first along the body diagonal and place it at a quarter distance along the body diagonal, I will get the diamond structure.

So, this diamond structure is generated by taking an FCC lattice; for example, here is an FCC lattice shown with the blue circles. You have this FCC cubic lattice. And I make another copy of this FCC cubic lattice which I just showed you. And if I move it along this body diagonal which is shown in red, and I place the second FCC lattice which has this green atoms at one quarter the distance along the body diagonal, then the lattice

which I generate is an FCC lattice. So, it is two interpenetrating FCC lattices that is your diamond structure.

Here I have drawn it with different colours just to identify and show you that I can make two FCC lattices interpenetrate each other. And here the diamond lattice is generated by these two interpenetrating lattices, where the movement of the second lattice with respect to the first is along the body diagonal and it sits at a quarter distance along the body diagonal ok. So, this point actually is sitting here ok. And then you have this complex distribution of atoms which can be nicely described by these two interpenetrating FCC lattices.

So, this is your diamond structure. The unit cell which is your conventional unit cell is simple cubic. And you define the simple cubic with two points per lattice. For this simple cubic cell, you will have two lattice points per cell. And those two points one is at $0, 0, 0$, which is this and the other one is that a by 4 , a by 4 , a by 4 , which is this. So, at every point, you are going to put at whichever point you will go to you have to put two lattice points per cell and you will generate your diamond lattice.

And diamond lattice is seen for silicon, germanium, these are very important semiconductors. And apart from diamond which is naturally from where the name the diamond lattice structure comes from, silicon and germanium also have this diamond lattice structure, which is this two interpenetrating FCC lattices which are displaced along the body diagonal.