Solid State Physics
Lecture 10
Brillouin zone for BCC and FCC Lattice

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So, after working out everything for the simple cubic lattice; let us consider a BCC lattice, a body centered cubic lattice. What is the reciprocal lattice to it? (Refer Slide Time: 00:42)

In order to find the reciprocal lattice, we need the real space lattice, the primitive lattice vectors $\overrightarrow{a_1}$ for BCC is given as $\frac{1}{2}a(-\hat{x}+\hat{y}+\hat{z})$; $\overrightarrow{a_2}$ is given as$\frac{1}{2}a(\hat{x}-\hat{y}+\hat{z})$; $\overrightarrow{a_3}$ is given as$\frac{1}{2}a(\hat{x}+\hat{y}-\hat{z})$. So, these are our primitive lattice vectors in the real space. Now, we need to find the cell volume that is $\overrightarrow{a_1}\cdot(\overrightarrow{a_2}\times\overrightarrow{a_3})$ and you have probably already worked it out and you have found it to be $\frac{1}{2}a^3$. With this and with our usual prescription for finding the reciprocal lattice vectors $\overrightarrow{b_1}$,$\overrightarrow{b_2}$ and $\overrightarrow{b_3}$; $\overrightarrow{b_1}$ would be given as $\frac{2\pi}{a}(\hat{y}+\hat{z})$, $\overrightarrow{b_2}$ given as $\frac{2\pi}{a}(\hat{x}+\hat{z})$, and $\overrightarrow{b_2}$ is given as $\frac{2\pi}{a}(\hat{x}+\hat{y})$. Does it ring a bell, are you familiar with these set of translation vectors? Certainly yes, this is along the direction of FCC lattice. So, these are the same as the direction of primitive lattice vectors for an FCC lattice, which means that the reciprocal lattice to BCC is FCC. We have found something very interesting and now comes the job of finding a Brillouin zone. (Refer Slide Time: 04:10)

So, in order to find the Brillouin zone, we need to define the $\overrightarrow{G}$ vectors, the reciprocal the translation vectors in reciprocal lattice, which is given as $v_1\overrightarrow{b_1}+v_2\overrightarrow{b_2}+v_3\overrightarrow{b_3}$. $v_1,/v_2,/v_3$ are as usual integers, which expressed in terms of a, that is the lattice constant in real space would be like $\frac{2\pi}{a}[(v_2+v_3)\hat{x}+(v_1+v_3)\hat{y}+(v_1+v_2)\hat{z}]$, this is the generic form of $\overrightarrow{G}$. So, the shortest $\overrightarrow{G}$ vectors would be that would be given as $\frac{2\pi}{a}(\pm\hat{y}\pm\hat{z})$, $\frac{2\pi}{a}(\pm\hat{x}\pm\hat{z})$ and $\frac{2\pi}{a}(\pm\hat{x}\pm\hat{y})$. So, in order to find the reciprocal unit cell, you need to create a parallel pipette using $\overrightarrow{b_1}$, $\overrightarrow{b_2}$ and $\overrightarrow{b_3}$. In order to find the first Brillouin zone, you need to find the planes that half these vectors; we have how many vectors here, each will give us with plus and minus sign here, each will give us four vectors and with this you will have many vectors, half them using planes and the smallest part, smallest volume that you cut out using that is the first Brillouin zone. Similarly with the second shortest $\overrightarrow{G}$ vectors you can find the second Brillouin zone, with the second third one you can find the third Brillouin zone and so on. You can see that the shape of the Brillouin zone in this case is going to be complicated; it would not be as simple as a cube or a parallel pipette, it would be more complicated than that. So, here is a homework for you; you need to draw the first Brillouin zone for a BCC lattice. I do not expect your drawing to be perfect, because as I already told that the picture is going to be really cumbersome; but give a thought to it and try to appreciate the geometry, try to construct something, so that you ah understand exactly what the Brillouin zone should look like. That is all about it; it is not about making a perfect drawing of it. And then after you have drawn something, look up the internet, try to see exactly how the Brillouin zone in case of ah BCC lattice looks like, that would be something really useful. Then let us move on to finding out the reciprocal lattice to FCC. Here I will do very little, it is your job to find out repeat the exercise that we have done so far. (Refer Slide Time: 08:26)

So, I will just tell you the primitive translation vectors that we have for FCC, I will just remind you here; $\overrightarrow{a_1}$ is given as $\frac{1}{2}a(\hat{y}+\hat{z})$, $\overrightarrow{a_2}$ equals$\frac{1}{2}a(\hat{x}+\hat{z})$ and $\overrightarrow{a_3}$ is $\frac{1}{2}a(\hat{x}+\hat{y})$. You need to find out the cell volume; the volume is given as $\overrightarrow{a_1}\cdot(\overrightarrow{a_2}\times\overrightarrow{a_3})$ and you have probably already worked it out and found $\frac{1}{4}a^3$, that is the cell volume here. So, your homework is to find $\overrightarrow{b_1}$, $\overrightarrow{b_2}$ and $\overrightarrow{b_3}$ the reciprocal axis vectors and also find the first Brillouin zone, draw the first Brillouin zone. I think you can already guess the answer to this part of the question, finding $\overrightarrow{b_1}$, $\overrightarrow{b_2}$ and $\overrightarrow{b_3}$; because when you considered BCC lattice, the reciprocal vectors were the primitive lattice vectors in real space for FCC. So, here it would be the other way around, for FCC it would become BCC; you can already guess that, it is just you need to work it out and show explicitly. And then drawing the first Brillouin zone again it is a cumbersome deal, it would not be simple; but you need to put some thought into it, you need to perform some exercise and then look up the internet to appreciate exactly how it should look like. That way you will understand the most of it.