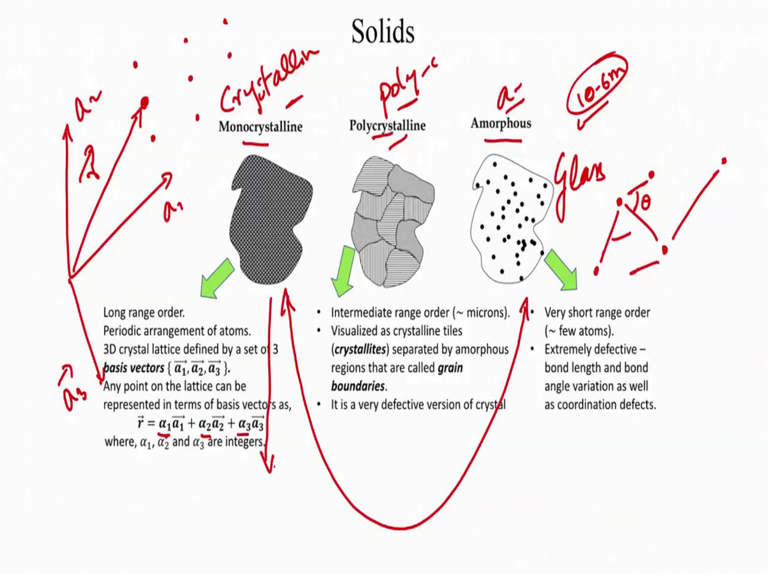
Semiconductor Devices and Circuits
Prof. Sanjiv Sambandan
Department of Instrumentation and Applied Physics
Indian Institute of Science, Bangalore

Lecture - 08
Solids: Crystals

(Refer Slide Time: 00:14)



Solids

Monocrystalline

Long range order.
Periodic arrangement of atoms.
3D crystal lattice defined by a set of 3 ***basis vectors*** $\{\vec{a_1}, \vec{a_2}, \vec{a_3}\}$.
Any point on the lattice can be represented in terms of basis vectors as,
$$\vec{r} = \alpha_1\vec{a_1} + \alpha_2\vec{a_2} + \alpha_3\vec{a_3}$$
where, α_1, α_2 and α_3 are integers.

Polycrystalline

- Intermediate range order (~ microns).
- Visualized as crystalline tiles (***crystallites***) separated by amorphous regions that are called ***grain boundaries***.
- It is a very defective version of crystal

Amorphous

- Very short range order (~ few atoms).
- Extremely defective – bond length and bond angle variation as well as coordination defects.

So, moving on. So, when you start bringing in many atoms close to each other then start creating solids, you could end up with different kinds of arrangements. And depending on the if you classify them in terms of their order of arrangements, you end up with things called as mono crystalline or crystalline solids, poly crystalline solids or amorphous solids ok. And what are these?

Crystalline solids are solids where the atoms are arranged periodically, throughout which means that for infinitely long distances there is complete periodicity in the arrangement, of the complete irregularity in the arrangement of atoms, they perfectly well arranged ok. So, if you look at the distance between these bonds it is all the same throughout ok.

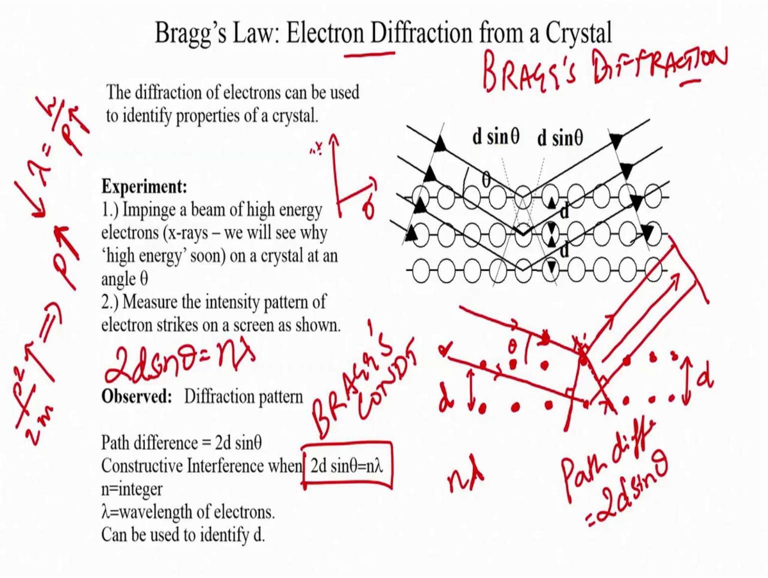
So, for example, this bond length will be the same between one plane to the other that bond length will be the same from one plane to the other etcetera. And in fact, they form such a nice grid of points that we could define a vector system or a coordinate system on this grid. So, if you if you were to define basis vectors, let us say a one a 2 and a 3 for a 3 dimensional space then any point on the any crystal or lattice point ok. So, this crystalline arrangement is something called as a lattice. And any atom occupying a lattice any lattice point which is basically an atom in the lattice, can be defined using these 3 orthogonal vectors ok. So, it is a linear combination of these vectors, where you have alpha 1, alpha 2, alpha 3 of constant coefficients. And this vector r is basically a linear combination of these orthogonal vectors. So, it is a very geometrically pleasing structure.

The poly crystalline structure is a little off, in the sense it is not that perfectly crystalline. The polycrystalline structure in fact, has got little tiles that are perfectly crystalline within the tile, and the size of each tile is the order of microns. So, let us say 10 microns. And you have different tiles, which have got which are within themselves crystalline, but the type of crystallinity changes. So, for example, the orientation of the crystalline cleans will be different ok. So, for example, within this little tile, this structure is perfectly crystalline, but the crystallinity holds true only for this distance of about a few microns.

And then you have another tile that starts and you have a different nature of crystallinity within the other tile. And these tiles are all separated these tiles are all called grains and these grains are all separated by grain boundaries ok. So, this is something called as a poly crystalline material and if you go to the other end of the spectrum. So, if we had crystalline and then we have poly crystalline which is somewhere in the middle the other end is a completely disordered structure, which is there is almost no periodicity at any scale level. And even if there is periodicity it is only of the order of a few atoms long and this is something called as an amorphous material. So, classic amorphous material is glass. So, these materials also called glasses.

So, in amorphous materials the atoms have no periodicity what is so ever. So, the bond lens between the different atoms will be different, their bond angles will be different and so on ok. So, it is a very extremely defective structure. And the and it is got immense consequences with regards to the distribution of energy levels, and you know the nature of band gaps etcetera and in our course we will look at crystalline materials ok.

(Refer Slide Time: 04:35)



Bragg's Law: Electron Diffraction from a Crystal

BRAGG'S DIFFRACTION

The diffraction of electrons can be used to identify properties of a crystal.

$\frac{p^2}{2m}\uparrow \Rightarrow p\uparrow \quad \downarrow\lambda = h/p\uparrow$

Experiment:

1.) Impinge a beam of high energy electrons (x-rays – we will see why 'high energy' soon) on a crystal at an angle θ

2.) Measure the intensity pattern of electron strikes on a screen as shown.

$2d\sin\theta = n\lambda$

BRAGG'S CONDⁿ

Observed: Diffraction pattern

Path difference = 2d sinθ

Constructive Interference when $\boxed{2d\sin\theta=n\lambda}$

n=integer

λ=wavelength of electrons.

Can be used to identify d.

it is helpful for us to study the geometry of these crystals. So, for example, let us study the distance between 2 crystal planes, which let us say is called d. Now a very powerful experimental technique to do that is something called as electron diffraction from a crystal or which is also called as Bragg's diffraction.

So, what is done is, the crystal is placed inside a system and the system puts out a very high energy electron beam, and makes it incident on the crystal. Let us say you have 2 rays of this beam ok. So, let me just turn draw this a little better. So, you have an high energy electron beam that is made incident on this crystal. And 2 rays of this incident and these of these beam tend to diffract because they are passing through this difference in the 2 lattice planes through this gap here, which is got a width of d. So, these electron beams are going to diffract and by placing a screen we would obtain an intensity pattern due to this diffraction. And by looking at this intensity pattern, one can identify whether this material is truly crystalline what the crystal spacing is etcetera.

So, firstly, let us just break down this entire experiment. So firstly, why do we need a high energy electron beam why cannot I just use visible light to study the distance between crystal plates. So, the crystal the distance between crystal planes the order is of the order of few angstroms ok. So, let us just say one e minus 10 meters. So, that is the order of the distance between the planes, but visible light has got a wave length which is about 4000 angstroms to about 7000 angstroms. So, it is about thousands of times larger than this distance. So, it is not possible for this large wavelength electromagnetic wave to resolve such a fine distance. And therefore, we need to use an electromagnetic wave which has got a wavelength of the order of one e minus 10 meters. And how is that done it is done by using an electron gun, for example, and firing the electrons off at very high momentum ok.

Because if you add a lot of energy to the electrons you increase the energy implies you increase the momentum and due to Bragg's law if an ink the momentum is increased the wavelength of the electrons will go down. And therefore, we can get very small wavelengths by having very large momentum in the electron beam. So, you use high energy electrons to study the crystal plane. So, this high energy electron is made incident on this plane. So, let us say the angle of incidence here is theta, it is not the angle of incidence, but it is the angle at which it abeyances off the plane it is theta. And you have your another ray which comes in like this ok. Now these 2 rays are going to interfere and create this intensity pattern.

Now, what is the condition for constructive interference? So, if you have let us say one wave that looks like this, and another that looks like this. So, let us just mark 2 points on this let us say A and B. So, since the peaks which are defined by A and B are at the same location, we could say that these in waves would interfere constructively. But now let us say we translate the second wave be translated by half a wavelength down. So, B now comes to this point. So, this is down by half a wavelength.

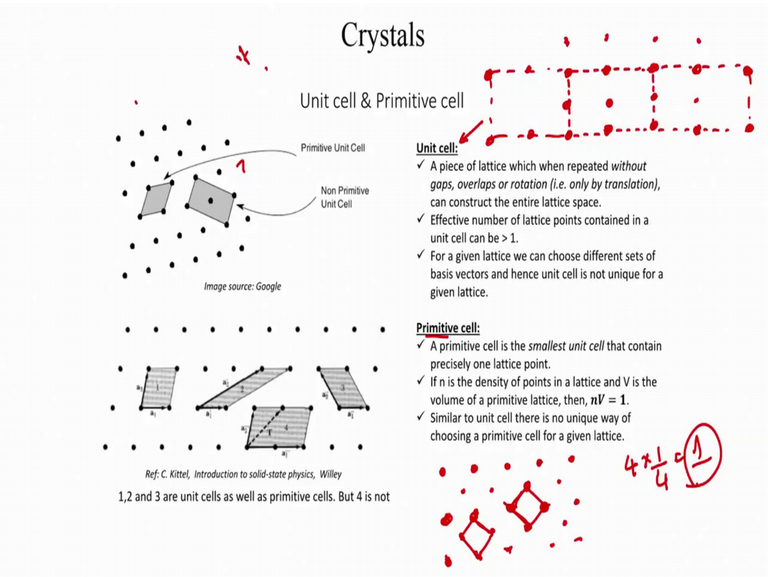
Now clearly the peak of this wave is at the same location as the valley of the other and therefore, you will have destructive interference. So now, if you translate this wave a little bit more by another half lambda, the peak of this wave has now shifted by another lambda by 2. And therefore, the distance the total translation has been one lambda that is one wavelength, and you will again have constructive interference.

So, you have constructive interference only when the path difference between the 2 waves or the if you want to think in terms of phase difference is also ok, but the path difference between the 2 waves should be an integer times lambda. It is only then that you will have constructive interference. So, what is the path difference between these 2 rays? So, let us draw a facet here you know it is sort of perpendicular to this and then other facet, or another plane here which is perpendicular. So, till this point both these rays travel the same distance exact same distance. And beyond this they are going to travel the exact same distance to the screen, but it is only this way, this ray has travelled a little more than the other in this region. So, this is the path difference this is the path difference between the 2 rays, it is only this little distance here and what is that distance.

So, we just use trigonometry to identify that. So, we have this little structure and this is the path difference. And the hypotenuse of these 2 triangles is d the crystal plane difference and you can easily find out that this is theta and therefore, this point this distance here is d sin theta, and that distance there is also d sin theta therefore, the total path difference is 2D sin theta. So, the condition for constructive interference is that 2D sin theta d equal to n times lambda ok.

So, that is that is given here. So, this is the condition for constructive interference and this is something called as the Bragg's condition. So, by keeping this crystal inside the system and by impinging an electron high energy electron beam on it, and by changing the value of theta one can get an intensity versus theta plot. And from that plot it is possible to identify whether the material is a crystalline material and you know if it is then what is the distance between the planes and etcetera. So, it is a very powerful tool to study crystals.

(Refer Slide Time: 12:30)



Crystals

Unit cell & Primitive cell

Image source: Google

Ref: C. Kittel, Introduction to solid-state physics, Willey

1,2 and 3 are unit cells as well as primitive cells. But 4 is not

Unit cell:

- ✓ A piece of lattice which when repeated *without gaps, overlaps or rotation (i.e. only by translation)*, can construct the entire lattice space.
- ✓ Effective number of lattice points contained in a unit cell can be > 1.
- ✓ For a given lattice we can choose different sets of basis vectors and hence unit cell is not unique for a given lattice.

Primitive cell:

- ✓ A primitive cell is the *smallest unit cell* that contain precisely one lattice point.
- ✓ If n is the density of points in a lattice and V is the volume of a primitive lattice, then, $nV = 1$.
- ✓ Similar to unit cell there is no unique way of choosing a primitive cell for a given lattice.

$4 \times \frac{1}{4} = \textcircled{1}$

So now coming to the defining the crystals themselves. So, we will just go through a few definitions it is not really fundamentally important from the point of view this course, but nevertheless it is useful to know these things. So, let us say you have a 2 dimensional crystal lattice as shown here ok. So, let me make something that is that is simple in case it is not visible. So, let us say you have a 2 dimensional crystal lattice. Now what are the different ways in which I can define this crystal space ok. So, the first thing is to identify the most fundamental structure that can define this crystal space. And there are 2 ways to go about it, the first is to define something called as a unit cell ok.

So, what is a unit cell a unit cell is essentially any building block that is composed of making a polygon let us say out of the out of these lattice points. Such that when this building block of in this geometrical entity is repeated again and again it can be used to fill up the entire lattice plane without having any gaps etcetera ok. So, this entity can be used to fill up entire lattice plane. So, for example, this could be a unit cell this could also be a unit cell. So, both these are possibilities for a unit cell. So, a unit cell is not unique you could have many units different kinds of unit cells. So, that is what a unit cell is. And if you want to locate the number of atoms in the unit cell, you know how many atoms are present in a unit cell what we have to do is we count the number of atoms and also watch out for the number of unit cells that are sharing those atoms ok. So, let us do an example and then it will become quite clear.

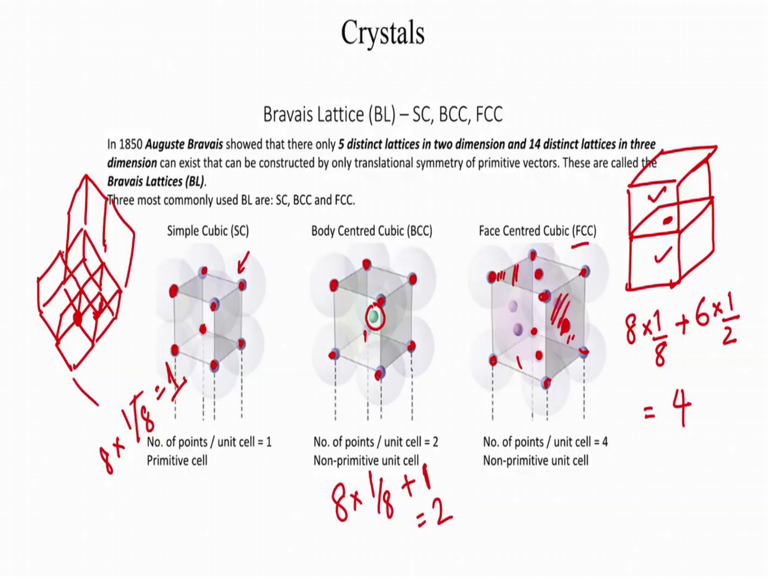
So, let us take a unit cell of this kind ok. So, it is you have you have a unit cell which is got a structure like this. So, this can be periodically used this can be used again and again to completely cover the entire lattice space. And your lattice space is composed of all these atoms which are drawn as these little solid circles. So, let us take this unit cell let me just fill up the space all around. So, that it becomes easier. So, let us take this unit cell. So, if you need to find out how many atoms are present in that unit cell, we see that there are 4 atoms of the vertices and there is one atom right here in the middle. So, therefore, it appears that there are 5 atoms, but then we need to be careful because this atom is already shared by 4-unit cell. So, this atom is equivalent to one 4th of an atom because it is shared by 4 unit cells. And how many of these kinds we have we have for such corner atoms we have this one we have this we have this in here.

So, we have 4 corner atoms vertex atoms and each of them are shared by 4 unit cells. And therefore, they are effectively one, but there is one in the middle which is shared by just one cell right, which is which only belongs to this particular unit cell and it is not shared by any cell. So, it is only belongs to that cell and therefore, there are total of 2 atoms in this unit cell ok. So, that is the way you calculate the total count and I think if you practice this you will obtain it or you will you will get better at this, but it is really not really important for this course, but nevertheless it is good to know.

Now, the other definition is something called as a primitive cell and what is the primitive cell a primitive cell is simply the smallest possible unit cell. Or if you want to quantify it the number of atoms in a primitive cell has to be one ok. So, for example, if you go back to our lattice we defined our unit cell as that and the number of atoms were 2, because there were 4 here and there is one in the middle. So, this cannot be a primitive cell a primitive cell has to be something smaller it has to be the smallest possible unit cell. And that is possible by having a unit cell that looks like this. For example,. So, if you have a unit cell that looks like this how many atoms does this unit cell have it has got 4 in the corner, but these 4 are shared by 4 other cells and therefore, there is a total of one atom per unit cell. So, this is a good definition of a primitive cell.

So, once again if you were to take a primitive cell, and tile up all the primitive cells next to each other you should be able to fill up the entire lattice space.

(Refer Slide Time: 17:44)



Crystals

Bravais Lattice (BL) – SC, BCC, FCC

In 1850 ***Auguste Bravais*** showed that there only ***5 distinct lattices in two dimension and 14 distinct lattices in three dimension*** can exist that can be constructed by only translational symmetry of primitive vectors. These are called the ***Bravais Lattices (BL)***.

Three most commonly used BL are: SC, BCC and FCC.

No. of points / unit cell = 1
Primitive cell

No. of points / unit cell = 2
Non-primitive unit cell

No. of points / unit cell = 4
Non-primitive unit cell

$8 \times 1/8 = 1$

$8 \times 1/8 + 1 = 2$

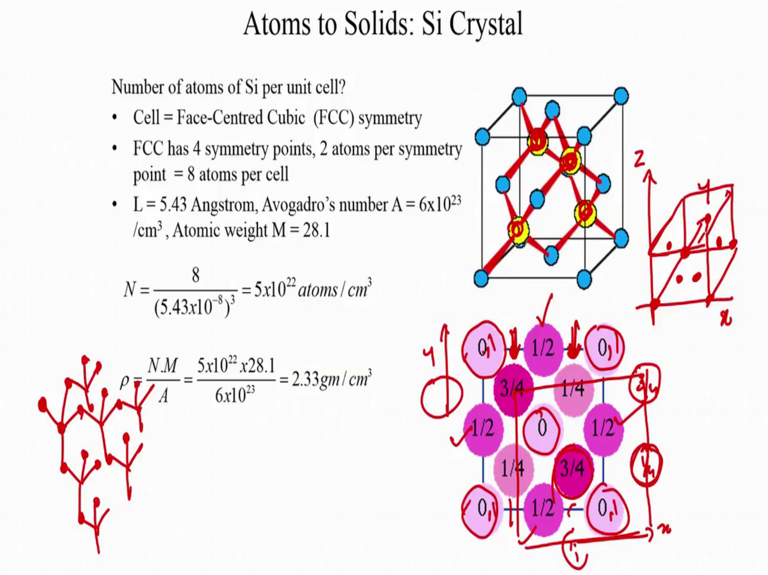
$8 \times \frac{1}{8} + 6 \times \frac{1}{2} = 4$

Now, heading towards 3D; so, if you go from 2D to 3D there are different kinds of lattice structures ok, and they can be classified in to very distinct types and there are basically 5 distinct classes for 2D lattices and there are 4, 14 distinct classes for 3 dimensional lattices and these are called as the Bravais lattices. So, some simple structures ok, which is useful to know for 3D are something called as a simple cubic the body centered cubic and the face centered cubic.

So, what is a simple cubic? A simple cubic is simply a cube with the atoms all sitting on the vertices of the cube. So now, if you have to go through your example and say identify the number of atoms. So, this is a one this is one kind of a 3 dimensional unit cell. So, what is the number of atoms in this 3D unit cell? It is you have 8 atoms on the vertices, but each of these atoms are shared by 8 other unit cells. And therefore, there is one effective cell per simple cubic unit cell. What about the body centered cubic? A body centered cubic has got 8 vertices just like the simple cubic structure, but it is also got one atom right inside the body. And therefore, the total number of atoms are going to be 8 into 1 by 8 plus that one which is not shared by any other cell.

So, which is 2 and the third is a face centered cubic structure, which is basically got your 8 corner atoms just like a simple cubic, but then on the centre of every face you also have one atom present. So, this is a side face and you have one that is a face on the table that is another and so on. So, what are the total number of atoms. So, if you think of this face atom it is going to be shared by 2 unit cells. So, you will have both these unit cells sharing that atom. So, you have 8 corner atoms shared by 8 unit cells, plus 6 face atoms shared by 2 unit cells. And therefore, you have a total of 4 atoms per face centered cubic unit cell.

(Refer Slide Time: 20:19)



Atoms to Solids: Si Crystal

Number of atoms of Si per unit cell?

- Cell = Face-Centred Cubic (FCC) symmetry
- FCC has 4 symmetry points, 2 atoms per symmetry point = 8 atoms per cell
- L = 5.43 Angstrom, Avogadro's number A = 6x10^{23} /cm^3, Atomic weight M = 28.1

$$N = \frac{8}{(5.43x10^{-8})^3} = 5x10^{22}\, atoms/cm^3$$

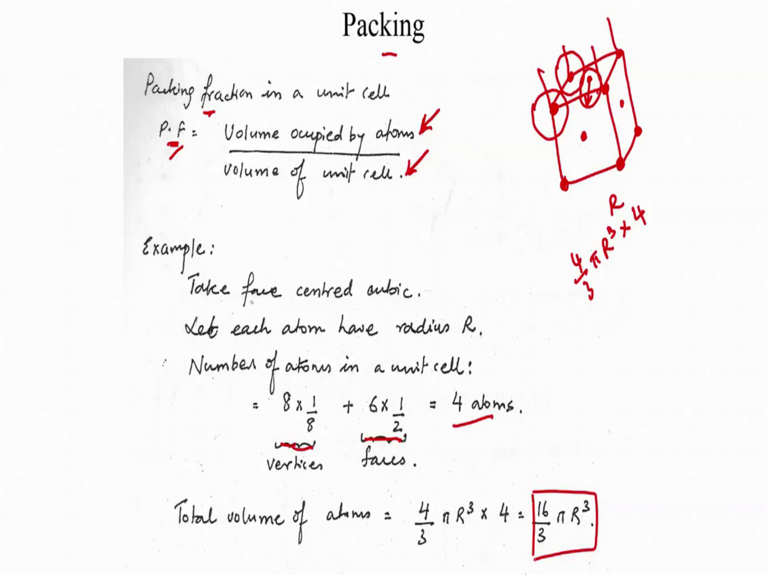
$$\rho = \frac{N.M}{A} = \frac{5x10^{22}\, x28.1}{6x10^{23}} = 2.33gm/cm^3$$

Now, particularly with regard to crystal silicon which is going to be our model of study, what is the silicon structure like you know just to just to give you an idea. So, here is a typo. So, you let us ignore that structure for now although the general geometry is correct, it looks like there are different kinds of atoms there. So, silicon structure only has silicon atoms and a simple way to draw it is it is basically 2 phase centered cubic structures which are sort of inter woven ok. And we will I will explain that, but a simple way to draw it is to simply draw a tetrahedral arrangement of atoms. And then continue drawing tetrahedral arrangements of atoms. So, you will end up with a diamond structure and then this will have it is own this will have it is own tetrahedron and so on.

So, that is the way you could you could possibly draw a silicon lattice, but then if you think of this picture here ok. So, what this picture tells you is you are looking at the silicon unit cell from the top ok, and these numbers that are written here I pointing out that there is an atom in that x and y. So, let us let us keep this as the y coordinate and the x coordinate. So, you are seeing x and y coordinate at the cell and this number here is the z coordinate of the system it is telling you the height of the atom from the floor. So, if you had to draw the say z, x and y what this is telling you is first let us look at these look at these 5 atoms ok. So, it is telling you that you have 5 atoms sitting right on the floor. And they are like a face centered cubic arrangement. And then let us look at these atoms which are on the sides.

So now we can construct the side walls that have got a certain height. And there are atoms sitting at the midpoint on these walls which are there on the side faces and this roof of the cell is basically the floor of the next cell. So, this structure repeats. So, this is at 0 1 the roof would be at one and therefore, it is a face centered cubic you see the first face centered cubic, but there is an also some of the atoms that we have not yet counted. So now, let us look at these atoms here the 3 by 4 the 1 by 4. If you were to sort of continue these atoms you will find that you know this arrangement can be extended throughout, and these are your other interwoven what you say face centered structures ok. So, you have these 2 interwoven arrangements that form your silicon lattice it is it is good to just spend some time and imagine it what we talk about.

(Refer Slide Time: 23:41)



Packing

Packing fraction in a unit cell

$$P.F = \frac{\text{Volume occupied by atoms}}{\text{volume of unit cell.}}$$

Example:

Take face centred cubic.

Let each atom have radius R.

Number of atoms in a unit cell:

$$= \underbrace{8 \times \frac{1}{8}}_{\text{vertices}} + \underbrace{6 \times \frac{1}{2}}_{\text{faces.}} = 4 \text{ atoms.}$$

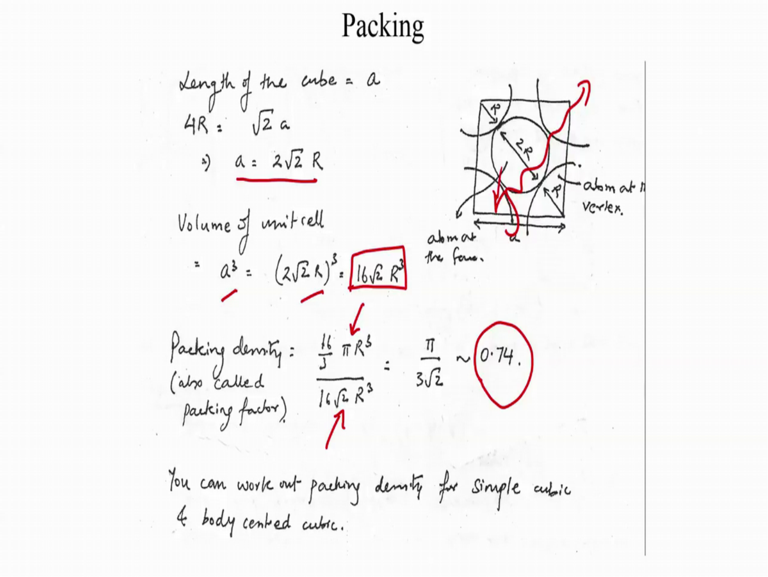
$$\text{Total volume of atoms} = \frac{4}{3}\pi R^3 \times 4 = \boxed{\frac{16}{3}\pi R^3}.$$

Now, is something called as a packing or the effectiveness of packing in a crystal. And in particular we define a factor called as a packing fraction in a crystal which tells you which gives you a ratio of the volume occupied by the atoms to the volume of the unit cell.

Now, the unit cell depending on the kind of a unit cell taken, and depending on the size of the atoms and their and the kind of and the kind of packing of these atoms, it is possible that there are some spaces in the unit cell or the volume of the unit cell might be larger than the effective volume of the atoms. Or you know the unit cell might be very efficiently packed. So, how does one determine you know this kind of the packing efficiency in unit cell? It is given by this packing fraction. So, let us just take an example and by just solving example you know the message of this packing fraction would be very, very clear.

So, let us take a face centered cubic. So, what is the face centered cubic you have a cubic unit cell you have 8 atoms on the vertices and on the centre of each phase you have a separate atom by itself. So, how many atoms do we have in this unit cell per unit cell, you have 8 corner atoms and each of these 8 atoms are shared by 8 other unit cells. And therefore, it is 8 into 1 by 8 plus 6 face atoms and each phase atom is shared by 2 unit cells and therefore, the 6 into 1 by 2 which is equal to 4 atoms. So, there are a total of 4 atoms per unit cell in the face centered cubic crystal, but now instead of just drawing the atoms as little dots let us actually define a radius for each atoms. Let us say that the each atom has got a radius which is which is got a radius of r. So, the volume of each atom is 4 by 3 pi r cube. And there are a total of 4 atoms an effect ml for effective number of atoms per unit cell. And therefore, the total volume of the atoms occupying this unit cell is 16 by 3 pi r cube.

(Refer Slide Time: 25:51)



Packing

Length of the cube = a

$4R = \sqrt{2}\,a$

$\Rightarrow \underline{a = 2\sqrt{2}\,R}$

Volume of unit cell

$= a^3 = (2\sqrt{2}\,R)^3 = \boxed{16\sqrt{2}\,R^3}$

Packing density (also called packing factor) : $\dfrac{\frac{16}{3}\pi R^3}{16\sqrt{2}\,R^3} = \dfrac{\pi}{3\sqrt{2}} \sim 0.74.$

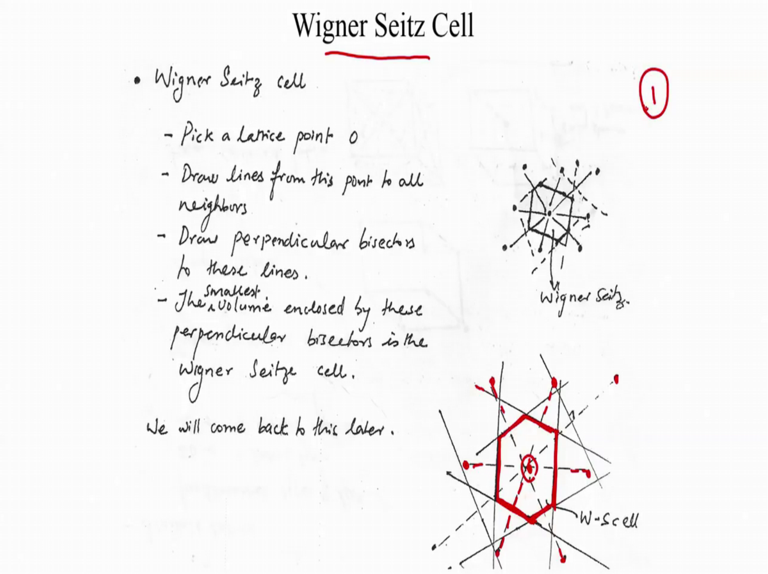
You can work out packing density for simple cubic & body centred cubic.

Now, so, let us draw this picture here. So, here is the top face of the cube. So, let us say the top face of this face centered cubic structure. So, you have one atom there and that is the next face centered cubic structure, you have another atom here you have yet another atom there. You have yet another atom here and that is your crystal structure. So, you are seeing the top of everything. So, if you look at only this unit cell you find that it is packed in this particular manner you have one face centered atom which has got which has got a diameter 2r. And you have all the other corner face centered cubic which are being shared which have all got an effective radius of r.

Now, therefore, given this definition of r, can given that all these atoms are not touching each other, and they have they have all packed into this unit cell in this particular manner. Can we define the length of the of this square what is this length a ok? So, what is a? A can be easily defined in terms of r, and you find that your A is nothing but 2 square root of 2 square root 2 of r. And therefore, the volume of the unit cell which is basically a cube of each side having length A is a cube. And a cube can be defined in terms of r because of this relation. So, you find that the volume of the unit cell is 16 square root 2 r cube and therefore, the packing density is the total volume of the atoms occupying this unit cell divided by the total volume of this cube and it turns out to be about 0.74 for a face centered cubic crystal. So, that is something called the packing density ok.

So, it is again something that is not going to be useful in this course, but having said that it is quite important because it determines. So, let us say this is the face across which you are going to have all your electron transport ok. So, let us say this is the face of the semiconductor on which you are having electron transport. So, this packing fraction determines the nature of the interaction of the electron with the crystal. So, the surface of the crystal and the arrangement of atoms on the surface of the crystal where the electron is going to move across does definitely impact the properties of the charge transport properties of charge transport and therefore, determines the current etcetera.

(Refer Slide Time: 28:32)



Wigner Seitz Cell

- Wigner Seitz cell
  - Pick a lattice point 0
  - Draw lines from this point to all neighbors
  - Draw perpendicular bisectors to these lines.
  - The smallest volume enclosed by these perpendicular bisectors is the Wigner Seitze cell.

We will come back to this later.

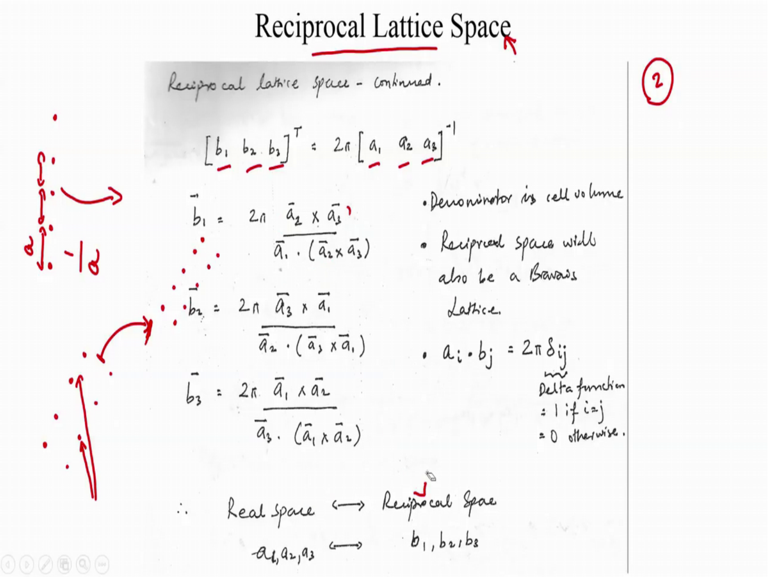
Now, we now come to the last bit of the course. And before we just drop off ok, I just want to define 3 ideas these ideas are again something that we will not be using in the rest of this course. So, it is all right for the students to completely skip these 3, but I feel that these are 3 critical ideas that provide a deeper insight. And the first idea is basically a geometrical construction. And it is something called as a Wigner Seitz cell. So, let us say you have and how do you how do you perform this geometrical constructions let us say you have a lattice ok. So, let us say these are the atoms of your lattice.

Now let us take any one atom in the lattice. So, let us take this particular atom here we will first draw lines, as shown by these dotted lines we will draw lines that connect this particular atom to the nearest neighbours. So, these are the nearest neighbour atoms and we are simply drawing lines that connect this atom to the nearest neighbours. So, that is the first step in this geometrical construction. Next what we do is we will draw the perpendicular bisectors to these lines. So, let us take this particular dotted line. So, what is the perpendicular bisector it is the line it is another line that divides this line 2 equal parts and intersects it at 90 degrees. So, we have that to be the perpendicular bisector to this particular line.

So, we now construct perpendicular bisectors to each of these dotted lines, that connect the atom that we have chosen to the nearest neighbouring atoms in the lattice. So, we have all these perpendicular bisectors that are shown here. And these perpendicular bisectors would all intersect they would all meet each other you see these bisectors. So, you see this bisector is meeting this one this bisector is meeting this one etcetera and all these perpendicular bisectors will therefore, enclose a certain space, you see there is there is if you were to draw this enclosure. So, which I am going to draw this very thick line here they would enclose this certain space. And they would basically create a cell ok. So, this enclosure by all these perpendicular bisectors creates this kind of a cell and this cell is something called as the Wigner Seitz cell.

So, you started off by taking picking an atom drawing lines to the nearest atoms constructing perpendicular bisectors and taking the inner shell that that is enveloped by all these perpendicular bisectors. So, this something called as a Wigner Seitz cell it is simply a construction, a geometrical construction. So, that is the first idea. Ok now this connects to another idea.

(Refer Slide Time: 31:31)



Reciprocal Lattice Space

Reciprocal lattice space - continued.

$$[b_1 \; b_2 \; b_3]^T = 2\pi [a_1 \; a_2 \; a_3]^{-1}$$

$$\vec{b}_1 = 2\pi \frac{\vec{a}_2 \times \vec{a}_3}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)}$$

$$\vec{b}_2 = 2\pi \frac{\vec{a}_3 \times \vec{a}_1}{\vec{a}_2 \cdot (\vec{a}_3 \times \vec{a}_1)}$$

$$\vec{b}_3 = 2\pi \frac{\vec{a}_1 \times \vec{a}_2}{\vec{a}_3 \cdot (\vec{a}_1 \times \vec{a}_2)}$$

- Denominator is cell volume
- Reciprocal space will also be a Bravais Lattice.
- $a_i \cdot b_j = 2\pi \delta_{ij}$

Delta function
$= 1$ if $i = j$
$= 0$ otherwise.

∴ Real space ⟷ Reciprocal Space

$a_1, a_2, a_3 \longleftrightarrow b_1, b_2, b_3$

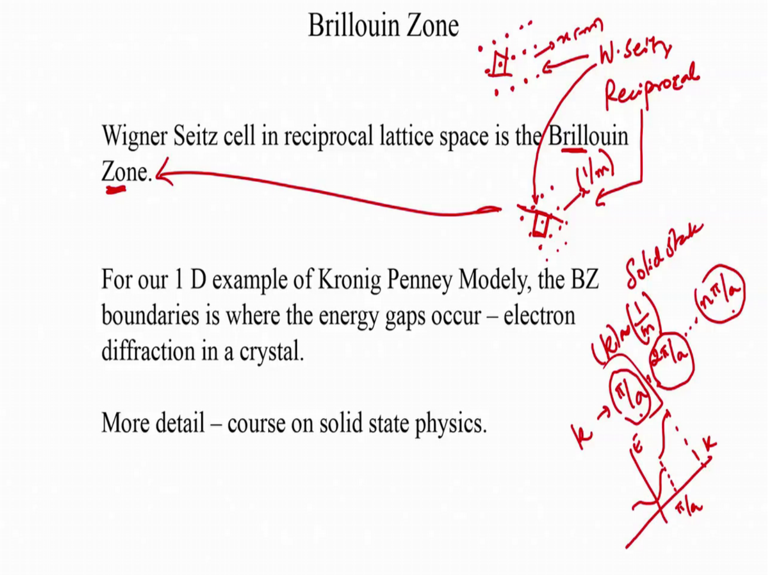
So, the second idea is something that is got to do with the reciprocal lattice space a very simply put you know do not worry about all these this mathematics. You can I will tell you what that is, but do not worry about it reciprocal lattice space is essentially a frequency space. So, let us say you have a periodic crystal you have got you have got atoms arranged in some period. So, it is got a periodic wavelength it is got some spatial period to it.

Now, what is the frequency it is essentially 1 by the spatial period. So, if it is a 1 by a could be considered to be the frequency. So, if you were to take the spatial Fourier transform of the real space you will end up with the in the frequency space and that frequency space is called as a reciprocal lattice space. So, as essentially a Fourier transform that connects the real space to the frequency space ok. So, essentially the idea behind what a reciprocal lattice spaces.

Now if you have a crystal if you have a perfect crystal in the real space and you take a Fourier transform you will end up with another with another periodic arrangement of points in the reciprocal lattice space, and that will also be a crystal. Although, it need not be the same kind of a crystal and the way you translate between real space to reciprocal lattice space is if you were to define basis vectors in the real space say a 1 a 2 and a 3. Such that any lattice point in the real space is a linear combination of these 3 orthogonal basis vectors. Then the reciprocal lattice space will also have basis vectors b 1, b 2, b 3 and they will all be connected to the real lattice space vectors in this particular fashion ok.

So, essentially you will find that in the 3D case it is basically this cross product divided by the volume of these cells was a very brief introduction to reciprocal lattice space.

(Refer Slide Time: 33:33)



Brillouin Zone

Wigner Seitz cell in reciprocal lattice space is the Brillouin Zone.

For our 1 D example of Kronig Penney Modely, the BZ boundaries is where the energy gaps occur – electron diffraction in a crystal.

More detail – course on solid state physics.

If you were to take these 2 ideas, you have the Wigner Seitz cell and you have the reciprocal lattice space and the reciprocal lattice space. So, Wigner Seitz cell was construct was a geometrical construct constructed on real lattice space. So, you took the lattice you had these lattice atoms. So, we are talking about real space which means x is measured in meters ok.

And we constructed a Wigner Seiz cell by drawing all these perpendicular bisectors in real lattice space and then we defined something called as a reciprocal lattice space, which is also a lattice, but it is all in 1 by meter ok. So, it is all the frequency domain it is the spatial frequency domain it is the dimensions are all 1 by meter and you have constructed another lattice here which is the reciprocal lattice.

Now, if you were to apply the same geometrical construct in a reciprocal lattice that is you construct a Wigner Seitz cell in a reciprocal lattice that enclosed boundary is something called as a Brillouin zone. Now the reason why I am introducing this topic is that these Brillouin zones you see these are all perpendicular bisectors ok, to these 2 pi by a 2 n pi by a lines. And therefore, this Brillouin zone facets occur at points where we are now in k space right we are in k space, we are all at you know 1 by meter that is the reciprocal or the frequency spatial frequency domain we are all in k space. So, the Brillouin zone boundaries occur at points where k is pi by a 2 pi by a and so on where integer times pi by a. So, that is where the Brillouin zones zone boundaries occur I am only talking about linear spatial thing linear arrangement of atoms.

So, if the Brillouin zone boundaries occur here, have you seen these points anywhere else? So, we have seen these points somewhere else and those were the points where the energy gaps occurred. So, when we drew the e k diagram after solving kronig's penney model we saw that the energy gaps or the discontinuities in energies occurred at pi by a 2 pi by a etcetera. So, therefore, the discontinuities are all occurring at the Brillouin zone boundaries. And it so, happens that the entire idea of this energy gap formation can also be explained by considering the diffraction of electrons at these facets ok. So, electrons reflect off these zone facets and therefore leads to the formation of energy gap.