

This video we cover the topics to be covered in module number 4. Title types of lattices, part one of the unit one title crystal structure. The outline of the presentation goes as follows. Important fundamental quantities, simple cubic structure, body centered, cubic structure, face centered cubic structure and site center cubic structure. Now. The students, after learning all these topics, they'll be able to differentiate between simple cubic, body centered cubic and face center cubic structures. They'll be able to determine coordination number of different cubic unit cells. They'll be able to determine relation between lattice constant and atomic radius. They'll be able to calculate atomic packing fraction of different cubic structures. Now these are the important fundamental quantities which we will be studying for every such crystal structure. Coordination number is defined as the number of equidistant nearest neighbors that an Atom has in a given crystal structure. Nearest neighbor distance is defined as the distance between the center of two nearest neighboring atoms. Atomic radius is defined as half the distance between the nearest neighbors in a crystalline solid without impurity. Atomic packing fraction is defined as a fraction of the space occupied by the atoms in a unit cell. Now to start, simple cubic structure. See, this is the cube. It has eight corners, so eight corners represent 8 lattice points and associated with each lattice point there is an atom. So this is the picture which showing you 8 atoms in a compact configuration placed at 8 lattice points and this figure represents the location of those eight lattice points. Now coming to the fact that we need to find out how many atoms are there in the unit cell? Let's do a calculation. Yeah, so there are eight atoms at 8 corner points and each lattice point will be shared by eight such unit cells, therefore, the Atom at this lattice point contributes one open eight part of it to a particular unit cell, and since eight such atoms are there, so eight into one upon 8, there are there is one Atom per unit cell of simple cubic structure. therefor it is called primitive Cell or primitive structure. Coordination number. Looking to the lattice point this point, this point is shared by 6. How? like this lattice point this side one this side one? This side one and this side one and up and down there for the coordination number becomes 6. Look into this diagram. A represents the lattice constant of the cubic structure, where r represents the radius of the Atom. It is very obvious from the geometry that a is equal to 2r. Coming to the atomic packing fraction volume of all atoms in the unit cell divided by volume of the unit cell. In the previous slide we have obtained, there is only one Atom per unit cell. Therefore, it is 1 into the volume of the Atom that is $\frac{4\pi}{3}r^3$ divided by the volume of the unit cell. That is a cube because the edge of each unit cell is a. So when we substitute the relation between a & r in this expression, we'll end up with 52%. That means the 52% of the volume is occupied by the atoms in that structure. Now coming to body centered cubic scale. Cubic structure. These elements listed here. They have body centered cubic structure and just like simple cubic structure, there are eight atoms at 8 corner points and there is one more Atom centrally placed in the inside the unit cell. So, the location of that centrally placed Atom is half in the X axis, Y axis half and Z axis half. Coming to let us calculate. How many atoms are there in a body centered cubic structure in itself? So already we had discussed in case of simple cubic structure, 8 corner atoms, this they contribute one open eight part of its to the particular unit cell and there are eight such 8 such Atom said there therefor 8 into one upon 8 plus the one which is inside the structure. So it is $1 + \frac{1}{2}$ two atoms per cell. So, body centered cubic scale. It is a non-primitive cell. Coordination number is 8 in this case. The coordination number is 8 because the body center Atom is touching all these eight corner atoms. Therefore, the coordination number is 8. Now look into this diagram. This cubic structure this site is a so also this side is a therefor the face diagonal is a upon root 2 and the body diagonal will be

a into $\sqrt{3}$ and there are atoms arranged in the body diagonal in this way. If you see it has a radius this is twice radius. This is one more so four times the radius of the Atom is nothing but. The body diagonal that is a into $\sqrt{3}$, therefore a can be written as $4r$ divided by $\sqrt{3}$. Now coming to atomic packing fraction, the definition remains same, but the volume of all items in the unit cell. Now since there are two atoms in the unit cell, it is 2 into $\frac{4}{3}\pi r^3$ divided by the volume of the cubic cell. And using the relation we obtained in the previous slide between a and r . If we replace it, we come down to 68%. Of the volume is occupied by the atoms in the body centered cubic structure. Next, let's go to face center cubic structure. The elements listed here have face centered cubic structure. And why it is called face centered? Apart from 8 corner lattice points if you see it has six surfaces yeah, up and down, left and right, front and back. And right in the middle of every face there is a lattice point or there is the Atom to be placed. So, this represents your face center cubic structure with atoms and the compact arrangement of the atoms, they touching each other. If you consider a surface or the face, say front face, we consider then let's see. Let's try to understand looking to this. There are four atoms at the four lattice points. Yeah, and there is this Atom at the middle of the surface. Yeah, so. If we have to figure it out that where are they are located? This tells you the locations of the face center atoms in the face center cubic structure. Now coming to the calculation of total number of atoms per unit cell, one upon 8 into 8 plus 6 into half, those at the contribution from the surface atoms give you 4 atoms per cell. Coordination number is 12. because if you take this in the XY plane, this one is sharing four atoms it is touching and YZ plane four atoms It is touching and ZX explain it is touching again four atoms. together it's coordination number is 12. And it is very easy to figure it out the surface diagonal being a into $\sqrt{2}$ that is equal to **FOUR** r . So therefore, we can write down a is equal to $2\sqrt{2}r$. And the Atom attracts packing fraction following the same principles. Since there are four atoms per units' cell, multiplying that with the volume of the Atom, dividing by the Volume of the unit cell. We get 74% of the volume is packed by the Atom. So from simple cubic body centered to face centered, we can make always a statement here that it is highly compact, highly compact in terms of the packing fraction now. Site centered cubic structure. If you see it has four lattice point as well as two lattice point on the two surface is therefore it has $1 + 1$ two lattice points per cell and coordination number is 6 just like simple cubic. With this we come to an end of module 4.