Introduction to Materials Science and Engineering

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Lecture - 34
ZnS

Let us consider the structure of cubic zinc sulfide also known as zinc blende.

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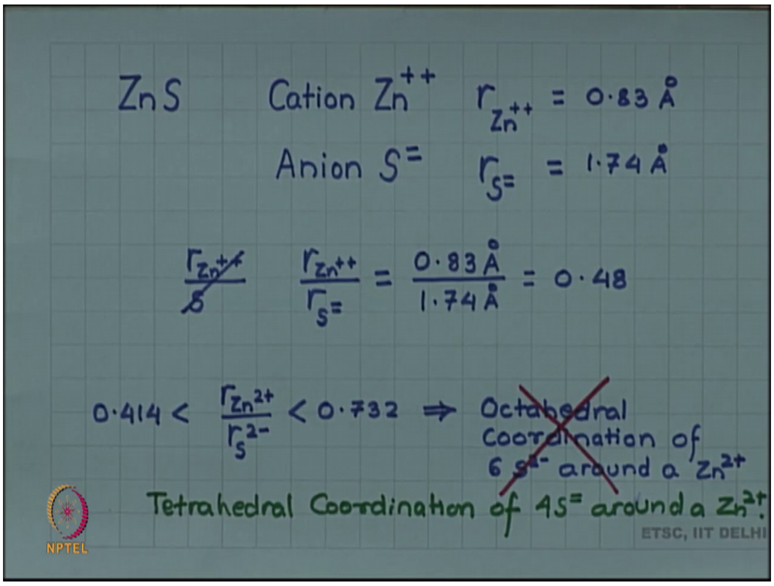

In this structure we have the cation zinc double plus 2 plus which has a ratio which has a radius of 0.83 angstrom anion, its sulfide anion with the radius of 1.74 angstrom. If we take the radius ratio we get a value of 0.48. This value comes between 0.414 and 0.731. So, this implies an octahedral coordination of 6 sulfide ions around a zinc cation. But in this case we are unfortunate this prediction turns out to be wrong. This is not the right prediction and the actual structure has a tetrahedral coordination tetrahedral coordination of four sulfide ions around a zinc cation.

So, this example, this counter example shows that radius ratio is actually a rule of thumb, it is not a some hard and fast rule which cannot be violated in some cases like in case of the zinc sulfide we do not get a structure which is predicted by the radius ratio instead we get a tetrahedral coordination of four sulfur around a zinc. What kind of a structure is this? So, let us look at this.

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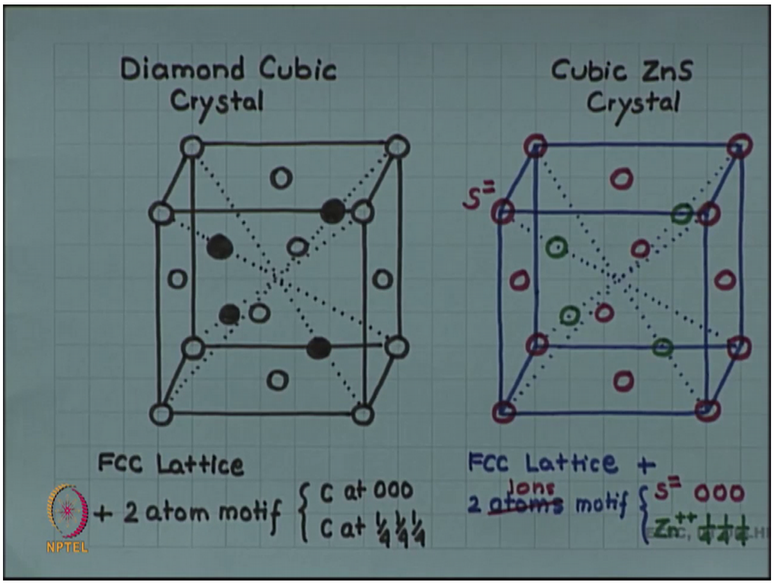

This structure can be related to the diamond cubic structure which we have studied before. So, the diamond cubic structure is an FCC lattice, but has two atom motif. So, the carbon atoms are at the FCC lattice points as I have already shown at the corners and face centers, but then there are 4 carbon atoms inside the unit cell which are sitting on one each on the body diagonals

So, there is a carbon atom here on this body diagonal and there is another carbon atom here on this body diagonal. On two body diagonals the carbon atoms are one-fourth up from the bottom. On the other two body diagonals the carbon atoms are three-fourth up from the bottom. So, these 4 inside carbon atoms although all of them are carbon, but let me shade the body diagonal ones just to emphasize that they are located on the body diagonal and this is how then, but both of them are carbon. So, in diamond cubic crystal diamond is anyway element all atoms are of the same type, but some are located on the face centered cubic site and on these body diagonals.

The cubic zinc sulphide structure can be related to this. So, the sulfide ions can now be made to sit on each of these face centered cubic site. So, I am placing the red sulfide ion first on the corners of the cube and then on the face centers the top and bottom face centers the left and right face centers and front and back face centers. So, this completes the locations of the sulfide ions, this is sulfide and the zinc ions are located exactly on the body diagonal just like in the case of diamond. So, on two body diagonals they are one-fourth up from the bottom in other two body diagonals they are three-fourth up from the bottom

So, the structure again is an the structure is again an FCC lattice and the motif is again of 2 atoms, the only difference is that now these 2 atoms are not of the same element they are of different element. I am writing atom, but when if you wish you can write it as ion. So, the sulfide ion is sitting at the lattice point whereas, the zinc ions now are located at the quarter quarter quarter site one-fourth, one-fourth, one-fourth. So, this is the cubic zinc sulfide crystal. Again these two structures should be considered as different crystal structure despite their similarity we will have diamond cubic crystal only if both the atoms are same. We will have a zinc sulfide structure if the two atoms are of different type the body diagonal ones and the corner and face center ones are different.

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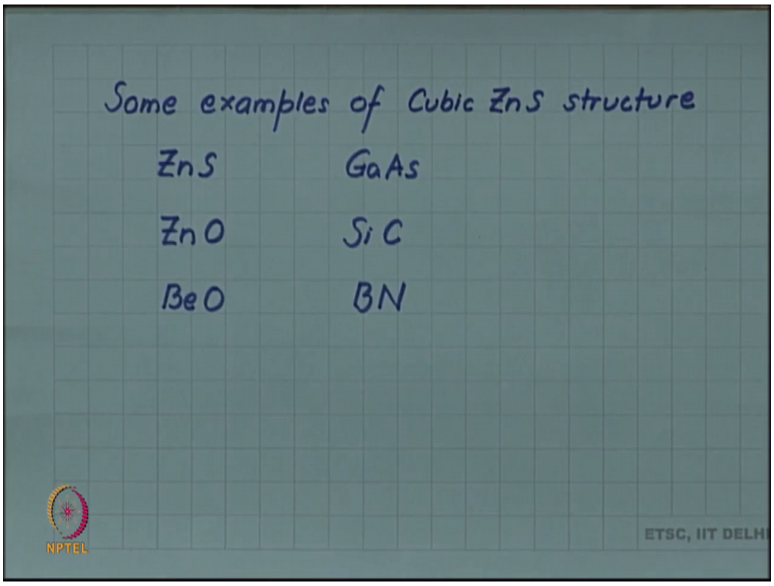

So, like other structures the cubic zinc sulfide also is a prototype structure and many other compounds many other equi atomic compound form cubic zinc sulfide structure. So, they are zinc oxide, beryllium oxide, gallium arsenide, silicon carbide, boron nitride among many others.