Introduction to Materials Science and Engineering
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Lecture - 32
NaCl

Let us look at, some examples of ionic solids which we have discussed. We discussed that, the radius ratio plays an important role in determining the structure of ionic solid.

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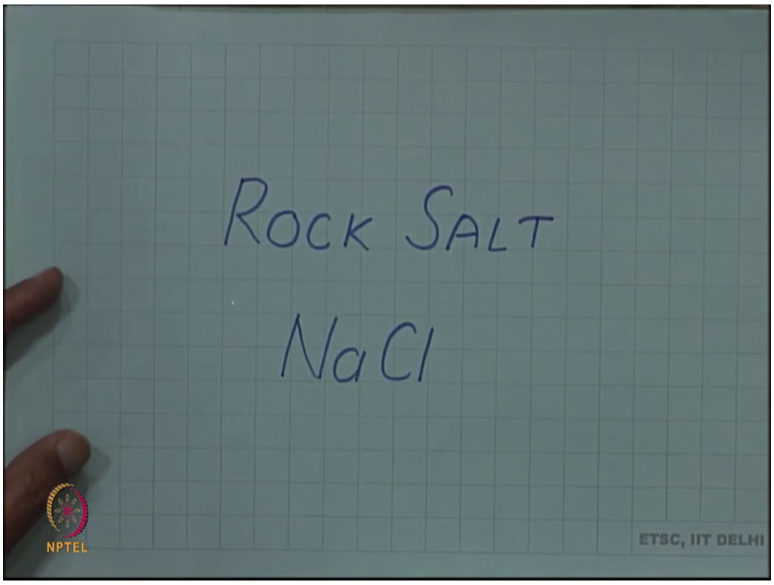

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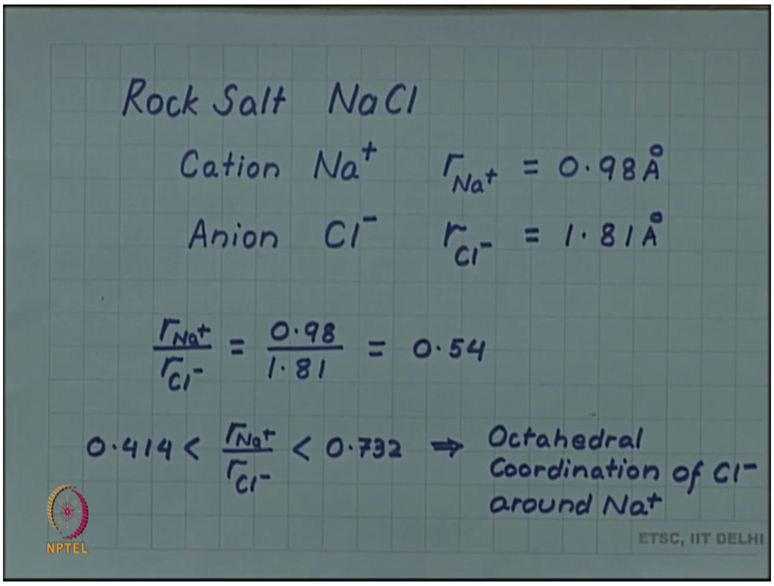

So, as a first example of our ionic solid, we take rock salt or sodium chloride. So, the sodium chloride the cation is Na plus, the sodium ion with the radius of 0.98 angstrom, the anion is chloride ion Cl minus with the radius of 1.81 angstrom. If we calculate the radius ratio, we get a value of 0.54. Now if we compare it, with the table given in a previously, we find that this radius ratio fits between 0.414 and 0.732.

So, this implies that there will be an octahedral coordination of chlorine or chloride ions around sodium plus. So, then octahedral coordination means, there will be 6 chloride ions around a single sodium ion.

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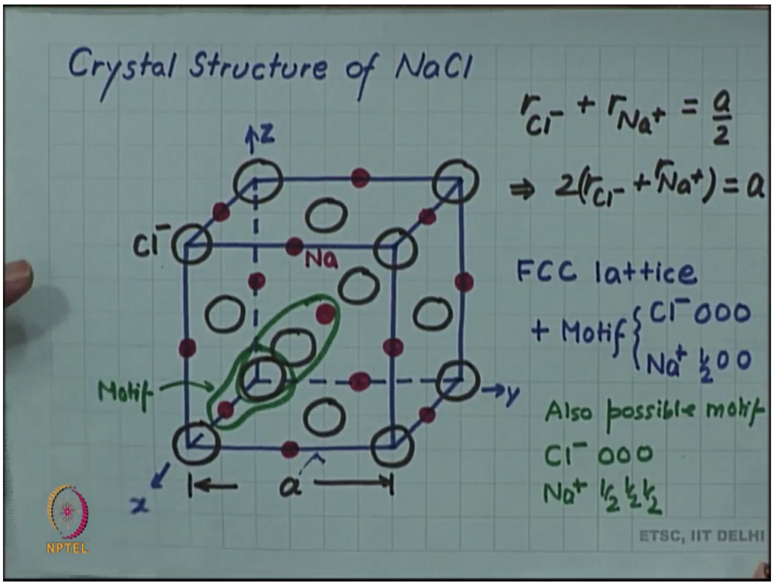

So, let us make the crystal structure of sodium chloride, notice that this radius ratio although, dictates the local coordination, this is the local coordination that there will be 6 chloride ions around one sodium ion. But, how they form? The real crystal structure cannot be decided by that. So, the real crystal structure has to be solved or has to be calculated separately and when it was solved by brag it was found that, in the real crystal structure chlorine ions form, the so, called face centered cubic sites.

So, on this in this cubic unit cell let me, place the chloride ions. So, these are the corners, then they are also on the face centers, left face, right face, top face and bottom face and then, we also have it on the front face and the back face. So, these are the 14 chloride ions in an fcc unit cell. The question is, where are the sodium ions? Now since sodium is having an octahedral coordination and you know that, the octahedral sites for face centered cubic is in the cube center as well as on the edge centers.

So, in fact, these are the locations where the sodium ion can fit having, an octahedral coordination. So, midpoints of all edges, and the center of the cube. So, if I put a sodium ion on each of these, my structure is complete. This is the sodium chloride crystal structure. I have of course, I am showing the ions are spaced out, in reality the closest ions will be touching. So, the chloride ion sitting on this corner and the sodium ion sitting here, along the edge these 2 ions are actually touching.

So, you can write the relationship between the radii and the lattice parameter. So, if the lattice parameter or the edge of the cube is a then, you can see the radius of the chloride ion, plus the radius of the sodium ion, should be equal to a by 2 or in other words 2 times the radius of chloride ion, plus the sodium ion, is equal to the lattice parameter a. Regarding the crystal structure, note that the chloride ions are forming an fcc structure.

So, this is the fcc lattice. So, the crystal structure is described as an face centered cubic lattice. But lattice is of course, only a set of points. So, you have to provide atoms to it, that is motif. So, motif will be of 2 atoms here, one is the chloride ion cl minus and that is at the origin, that is that each lattice not the origin, at each lattice point these are the displacement coordinates with respect to the lattice points. So, with respect to each lattice point, without any displacement chloride ions are put. So, that is a face centered cubic lattice sites corners and face centers.

So, we have the chloride ion and, but this will not give me the sodium chloride structure, I need sodium also. So, I have to take one sodium ion also in the motif. So, you have to take the sodium ion in the motif and this will then complete the motif. The sodium ion you can select, the nearest sodium ion which will be along let us say if, this is the x y or z. So, you can select your motif, by selecting a nearest sodium ion along the x axis. So, this can be your a possible motif. So, sodium ion you can then write as half at half oo, but sometimes this appears that the x axis neighbor is being given preference over other neighbors, there is an neighbor at on the y axis also at the same distance and the z axis also at the same distance.

So, sometimes some authors feel that it is better to take, a motif which is the chloride ion, also possible motif, another choice of motif is chloride ion at ooo, but sodium ion at half, half, half. So, although this sodium and is not nearest to this chloride ion, but this has symmetric coordinates with respect to x y and z. So, in that sense it appears better to select, the central atom or the central ion as, the part of motif.

It should be noted that sodium chloride structure is not just the structure of sodium chloride, but it is a prototype structure. Any ab compound where a is in cation and b is anion. So, any such equi atomic compounds ab, which will have this kind of a structure that, the cube corners and face centers are taken by the anions and edge centers and the body centers are taken by cation any such structure will be called a sodium chloride structure.

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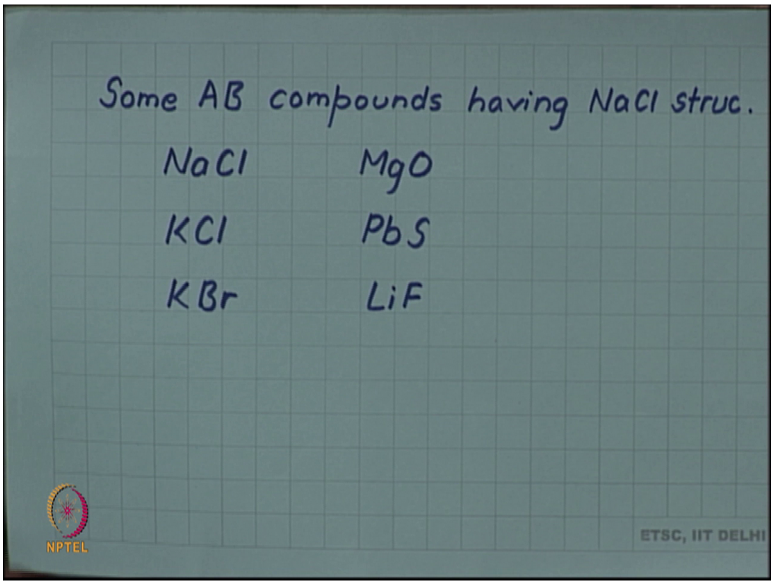

Sodium chloride structure is not only the structure of sodium chloride, but many such compounds for example, magnesium oxide, potassium chloride, lead sulfide, potassium bromide and lithium fluoride. Many such examples of sodium chloride structure is available in nature this is only a partial set.