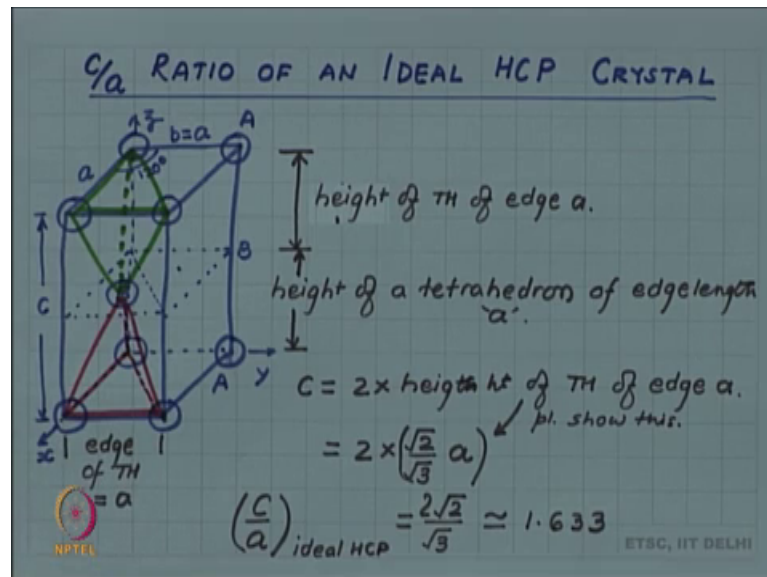


Introduction to Materials Science and Engineering
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Lecture – 19
C/a ratio of an ideal HCP crystal

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Today let us look at c by a ratio of an ideal HCP crystal. C by a ratio is an important parameter for hexagonal close packed structure, as we have seen that the hexagonal unit cell let me try to draw the hexagonal unit cell is a rhombus-based prism. So, the base of hexagonal close packed crystal, the unit cell at the base of the unit cell is a rhombus a equal b and gamma equal to 120 degree.

So, 120 degree rhombus is what defines the base of the unit cell and then it is a prism based on this rhombus; what tried to draw the unit cell this is the x axis, this will be the y axis, and this is the z axis, this included angle between x and y axis is 120 degree, and this is a and b is equal to a, and the height of the unit cell is what is called the c parameter, and when we are talking of the c by a ratio we are talking about the ratio of this c to this a. Now in a normal hexagonal unit cell the c and a can have any value and c by a ratio, can have any value based on hexagonal symmetry there is no restriction, but hexagonal close packed crystal is a special structure as we have seen with the a b stacking sequence of atoms.

So, the a atoms are the atoms located at the corners of the unit cells. So, these are all A atoms and on the top corner these atoms are also A atoms. So, the c parameter is essentially a spacing between 2 successive a planes; however, note that there is an intermediate plane which is the b plane, you have an intermediate plane.

Just midway between these 2 a planes which is the b plane, because the stacking sequence of hexagonal close packed structure is a b a b, the location of the b atom in this plane can be obtained by dividing this rhombus the mid rhombus, into 2 equilateral triangles and one of these triangles is designated as b, another one is designated as c. So, in the centroid of b triangle if I place an atom that is what is the B atom, and this is a B plane. So now, I have completed the unit cell all the atoms are shown, rhombus-based prism height c, a b a b stacking a 2 a c, and a mid plane atom B is there right inside the unit cell.

Now, notice that and we have discussed this, that this b atom is actually sitting on the 3 a atoms below. So, with respect to these 3 a atoms, this b atom is forming a tetrahedron, an upright tetrahedron is formed if I join the 3 atoms below on which this b atom is sitting. So, I have an upright tetrahedron here shown in red, but the same b atom also forms a tetrahedron with the 3 a atoms above it, this forms an inverted tetrahedron if I now join this p atom to these atoms above, then here also it forms a tetrahedron only it is an upside down tetrahedron. So, what we call an inverted tetrahedron.

So now you can easily see that a to b distance is height of a tetrahedron, and what is the edge length of the tetrahedron? That is the lattice parameter a. So, edge of the tetrahedron is nothing but a. So, height of a tetrahedron I can say height of a tetrahedron of edge length a, and this of course, is again the same height, the inverted tetrahedron is identical to the upright tetrahedron and has the same height.

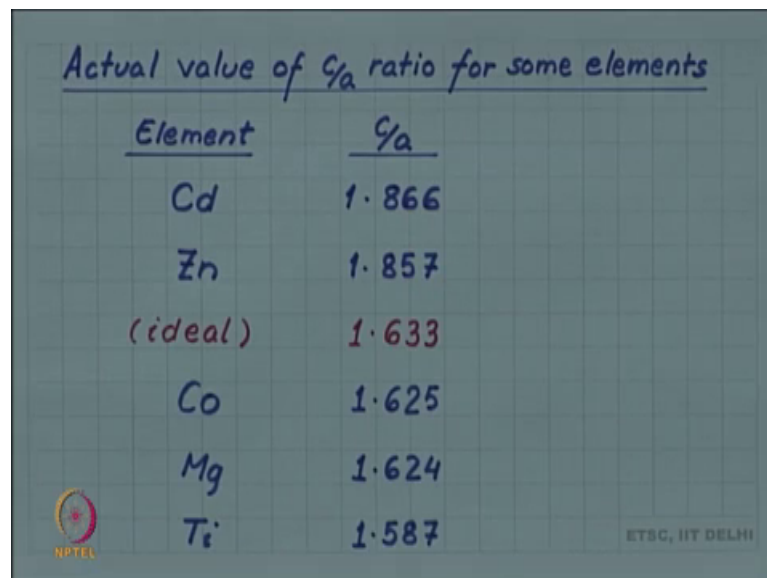
So, this is also height of tetrahedron of edge a. Which means now a to a since a to a distance is what is c, we have a simple relation that c is nothing but 2 times the height of this tetrahedron, height of tetrahedron of edge a, and if you try to work out I leave this exercise for you if you try to work out what is the height of a tetrahedron of edge length a, you will find that this comes out to be $\frac{\sqrt{2}}{\sqrt{3}} a$.

So, from this. So, this $\frac{\sqrt{2}}{\sqrt{3}} a$ is what is the height of this tetrahedron. This I am leaving this as an exercise for you please show this. So, what you get now if I now

try to find c by a and this we call the c by a for ideal h c p, this becomes $2\sqrt{2}$ by $\sqrt{3}$ or if you calculate it up the approximate value will be 1.633. So, it is easy to calculate, but this is what one will get. So, a hexagonal a normal hexagonal crystal can have any c by a ratio, but an ideal hexagonal close packed crystal, will always have this c by a ratio.

So, let us look at the values of c by a ratio in actual elements.

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Actual value of c/a ratio for some elements

Element	c/a
Cd	1.866
Zn	1.857
(ideal)	1.633
Co	1.625
Mg	1.624
Ti	1.587

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So, the ideal value is shown here 1.633, you can see that some element like cadmium zinc have values significantly higher than the ideal value, cadmium has 1.866, zinc is 1.857. So, both these elements have c by a ratio significantly higher than the ideal value, similarly there are elements like cobalt magnesium and titanium which have values lower than the ideal value, cobalt and magnesium are rather close they are lower, but rather close to the ideal value, but titanium is significantly lower than the ideal value. So, real element do not actually form exactly ideal structure.

So, ideal structure is a model structure to which the real elements try to approximate. So, we called all of them a hexagonal close packed structure, but they are not ideally hexagonal close packed. So, with this we will end the topic of hexagonal close packed structure, and in the next lecture we will take up cubic close packed that was another closed packing as you remember, the other close packed structure was the cubic close packed structure with a stacking sequence a b c a b c. So, we will take that topic in the next lecture.