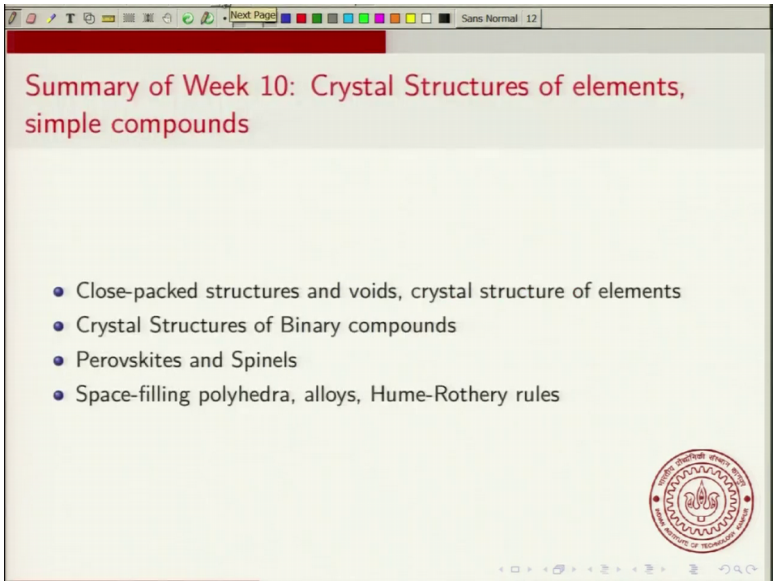
Solid State Chemistry
Prof. Madhav Ranganathan
Department of Chemistry
Indian Institute of Technology, Kanpur

Lecture - 50
Summary of Week 10, Practice Questions

In the last lecture of week 10, I will summarize what we have learnt in week 10 and do some practice problems. So, week 10, lecture 5 will be summary of week 10 and practice problems. So, what did we learn in week 10?

(Refer Slide Time: 00:32)

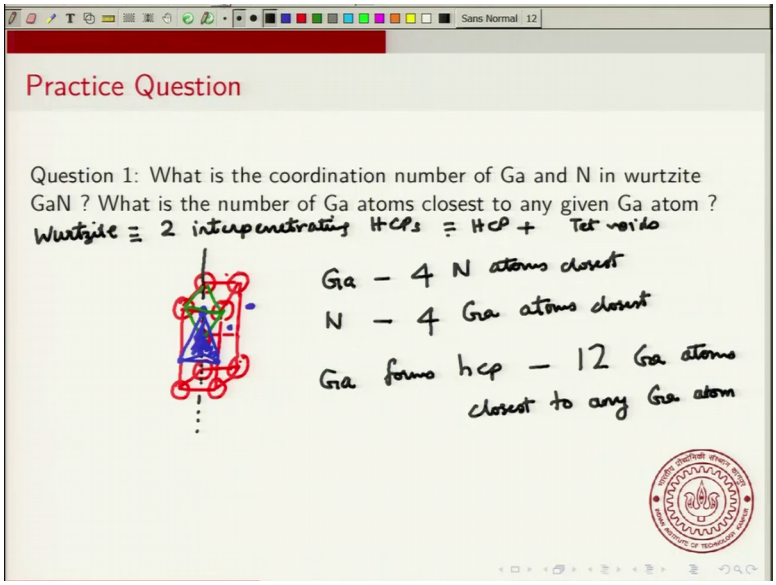


In week 10 we learnt about the crystal structures of elements and simple compounds ok. So, we first saw, we first looked at close packed structures and voids ok, and we understood where the octahedral and tetrahedral voids come in close packed structures ok. And then we looked at the crystal structure of elements, then we saw crystal structures of binary compounds, we looked at several binary compounds and we saw their crystal structures. Then I looked at two interesting ternary compounds ok; these are Perovskites and Spinels and we saw their structures. And then finally, we I discussed a concept of space filling polyhedral, alloys and we looked at Hume-Rothery rules ok.

So, now I will go to a couple of practice questions. I mean in this week I want to emphasize that you know there are not really too many, I mean most of it is descriptive,

so the questions will be mainly related to things like coordination number or calculations of distances, but most of the other concepts are fairly descriptive ok.

(Refer Slide Time: 01:44)



So, this is a question, what is the coordination number of gallium and nitrogen in wurtzite GaN ok, and what are the number of gallium atoms closest to any gallium atom ok. Now the wurtzite crystal structure is essentially two interpenetrating HCPs.

So, you can look at it as two inter penetrating HCPs ok, or you can, alternatively you can look at it as HCP plus tetrahedral voids. And you can already see, you know the moment you say half of tetrahedral voids you immediately realize what the coordination number is ok. So, in this, you can think of the gallium atom as occupying the tetrahedral voids, not of it is just, we will just say tetrahedral voids.

So, now, what is the, what will this structure look like? So, if you have an HCP ok. Then let me show the sulfide ions in red, and I am deliberately not showing them, touching each other. And now this is the hexagonal cell, and then in an HCP you have an additional sulphide and located here ok.

So, these are the, these are the locations of the of the sulfur sulfurs. And the gallium, gallium, we can choose the location, so we can choose whichever tetrahedral voids we want them to occupy, but definitely there is a tetrahedral void in the right here ok, which,

so I will put a gallium write here. And this will be directly above this, above this sulfide ion ok. And actually it will this goes somewhere here comes out ok.

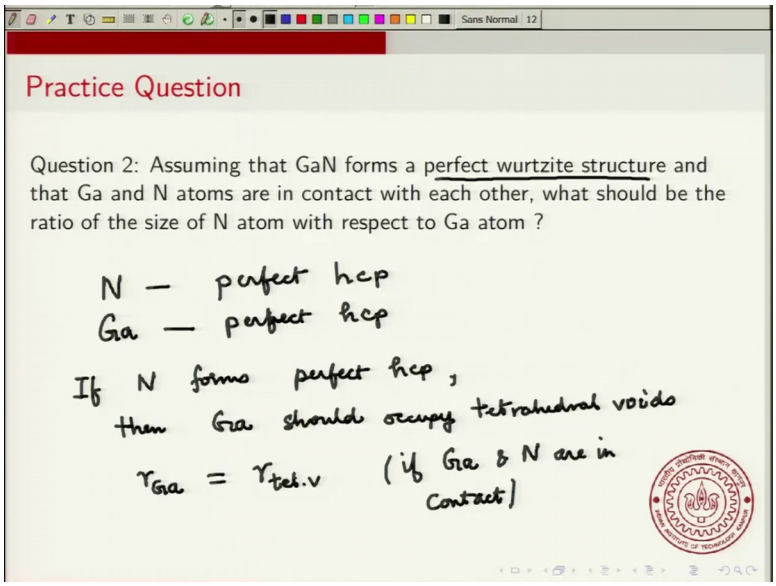
So, that is the location of the tetrahedral void. It comes out right in between these 3 goes on. So, the gallium is located right in this void ok, which is actually in the coordination polyhedron is, basically it is closest to these four, so that is the tetrahedron of coordination ok. So, now what is the coordination number of, what is the coordination number of gallium and nitrogen ok?

So, clearly gallium is 4 coordinated and since these are 2 interpenetrating HCPs ok, then the gallium will also form an HCP. So, the gallium will also form an HCP. In this case it will be there will also be gallium atoms here, here and then it will end, the hole here and here, and this HCP will extend ok. You will additionally, you will also have some gallium atoms that are that are right about these ok.

So, you will also have. No not this one, you will also have gallium atoms that are here ok and so you can see the. Now I am showing the coordination polyhedra for this for this nitrogen atom and that is also 4. So, nitrogen also has coordination number of 4. Now the next question is, what is the number of gallium atoms closest to any gallium atom ok. Now this answer can be this can be answered very easily. So, since gallium forms HCP ok, the answer is just 12 gallium atoms closest to any gallium atom ok.

So, if you look and similar similarly for nitrogen also. So, if you look at any gallium atom ok, there will be 4 nitrogen's that are closest to it ok. So, 4, so these the coordination on are number 4 relates to the 4 nitrogen atoms that are closest to it ok. And the nitrogen atom has 4 gallium atoms that are closest to it, but if you look at gallium what are the gallium atoms that are close to it, then the answer is 12 ok. So, there are 12 gallium atoms closest to anyone, any given gallium atom ok.

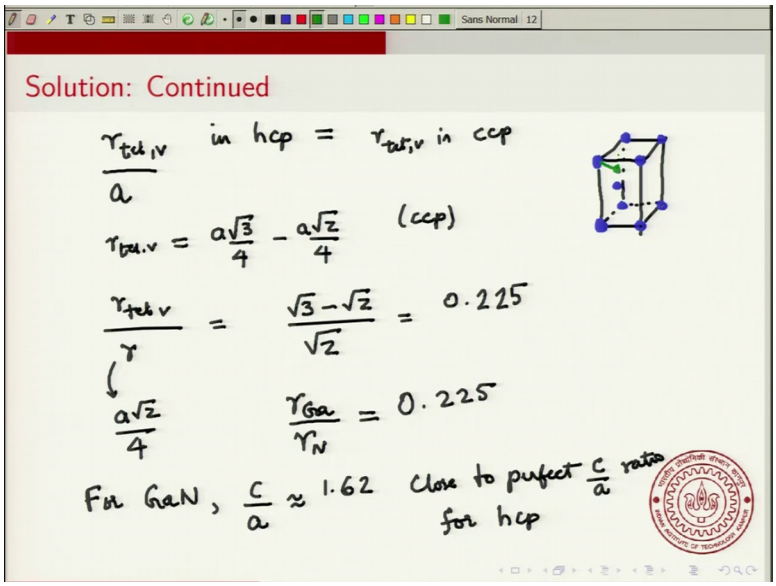
(Refer Slide Time: 08:15)



The next practice question is, suppose you assume that gallium nitride forms a perfect wurtzite structure and that gallium and nitrogen atoms are in contact with each other, what should be the ratio of the size of nitrogen atom with respect to gallium atom ok. So, this question can be answered in a few different ways, but let me mention a few things. So, the perfect wurtzite structure, perfect wurtzite structure, means gallium or I will start with nitrogen forms a perfect HCP, and so does gallium, so the individual gallium and nitrogen ok.

Let me write it separately, so gallium, the individual gallium on nitrogen's they form perfect HCP ok. And so, what should be the ratio of size of nitrogen atom with respect to gallium atom ok? So, again you can do this very easily. So, let us say we take the nitrogen as a larger atom ok. So, if perfect HCP ok, then gallium should occupy tetrahedral voids ok. So, if nitrogen forms a perfect HCP then the gallium should occupy the tetrahedral voids ok. And so, therefore, therefore, radius of gallium should be equal to radius of tetrahedral voids ok. This is the radius of the tetrahedral void if gallium and nitrogen are in contact ok. So, if they are perfectly touching each other then the radius of the gallium should be exactly be equal to the radius of the tetrahedral void ok.

(Refer Slide Time: 10:43)



So, now the radius of the tetrahedral void in gallium ok, if this is, this in HCP is equal to radius of tetra, or the in terms of divided by the lattice parameter a in HCP is equal to radius of tetrahedral void in ccp ok. And you, we also have seen ok, so this turns out to be 2 by 4. This is in the case of in the case of ccp and if I take r tetrahedral void divided by r of the of the larger atoms ok.

So, that it, that becomes the root 3 minus root 2 divided by root 2 ok, because the radius of radius of nitrogen ok, the larger, this is the radius of the larger species, so r equal to a root 2 by 4 ok, and this is equal to 0.22, about 0.225 ok. So, what you would expect? So, ideally you would want radius of gallium divided by radius of nitrogen should be equal to 0.225 ok. If the nitrogen forms a perfect HCP and the gallium also forms a perfect HCP and both of them form a perfect wurtzite structure. Now of course, this ratio is not, this ratio is not exactly satisfied, but it turns out that the that the that for gallium nitride ok, the c by a ratio is very close to, very close to 1.62 which is very, which is very close to the close to perfect ratio c by a ratio for HCP.

So, for an ideal HCP the c by a ratio is about 1.63 and this about 1.62, which is very close to that ok. and I took the, I took the liberty of using the tetrahedral void in the cubic close packed to estimate this ok, but you can also do this for the hexagonal close packed and you will get exactly the same answer.

So, we can just use the HCP structure and locate the tetrahedral void. In this case the geometry is slightly more involved, so just to illustrate you have the hexagonal close packed structure ok. This is the, this is the unit cell and the tetrahedral void is located right here ok. And you can, now in a HCP additionally, you have a you also have an atom here.

So, let me show all these atoms in blue and you have an atom here, and the tetrahedral void is directly above or below whichever way you want to show this ok, this atom. And so and so you can you can determine the, you can determine this radius of tetrahedral void by geometric analysis of this void and you will get exactly the same ratio ok.

So, with this I will conclude this lecture, and I will also conclude week 10 of this course. And as I had mentioned earlier that in this week we sort of saw how all that we learnt about symmetry, packing, crystal structures ok, all that is used to describe the structures of real materials ok. And how all the language that we learnt in the previous 9 weeks ok, we put it to use in describing the structures of several materials. And as I said a lot of the material is very descriptive, so I do not expect you to memorize too many things ok, but at least some basic concepts of this of these structures of solids you should have ok. So.

Thank you.