Solid State Chemistry
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Lecture – 10
Summary of Week 2, Practice Problems

Now, we will go to the fifth lecture or the last lecture of the second week. And in this lecture, I will essentially review what we learnt during this week very briefly and also do a couple of questions, ok. So, let us go to the lecture.

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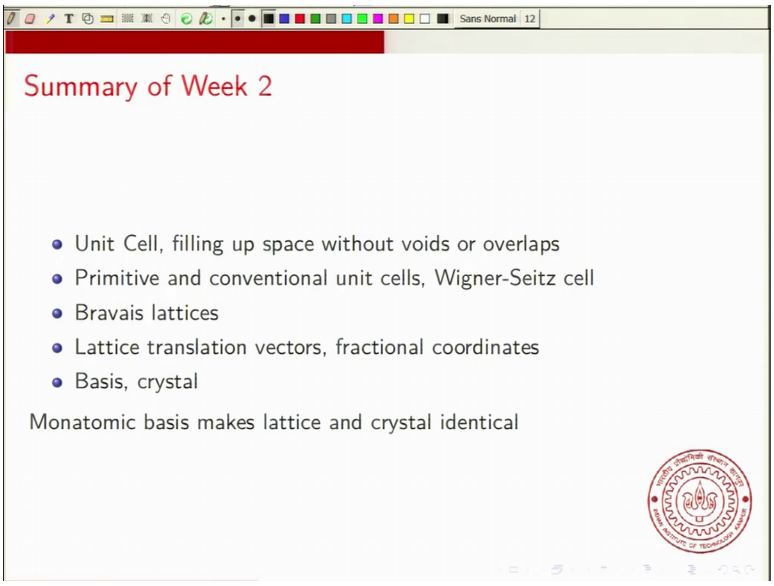

In week 2, you learnt we learnt first about a unit cell, we learnt the concept that the unit cell should fill up space without voids or overlaps, we learnt about the primitive and conventional unit cells, and we also saw how to construct a Wigner-Seitz cell. A Wigner-Seitz cell is a unit cell that contains exactly one point and it has the entire symmetry of the crystal.

Then we learnt about Bravais lattices, we saw Bravais lattices in two-dimensions, Bravais lattices in three-dimensions and then we learnt about the concept of lattice translation vectors and that of fractional coordinates. And finally, we saw how a crystal is formed using a lattice and a basis, ok. And again, I did not emphasize this, but if you have a monatomic basis if you have a just a single atom basis. So, a lattice with just a single atom basis we will basically make the crystal and the lattice identical, identical to each other, ok.

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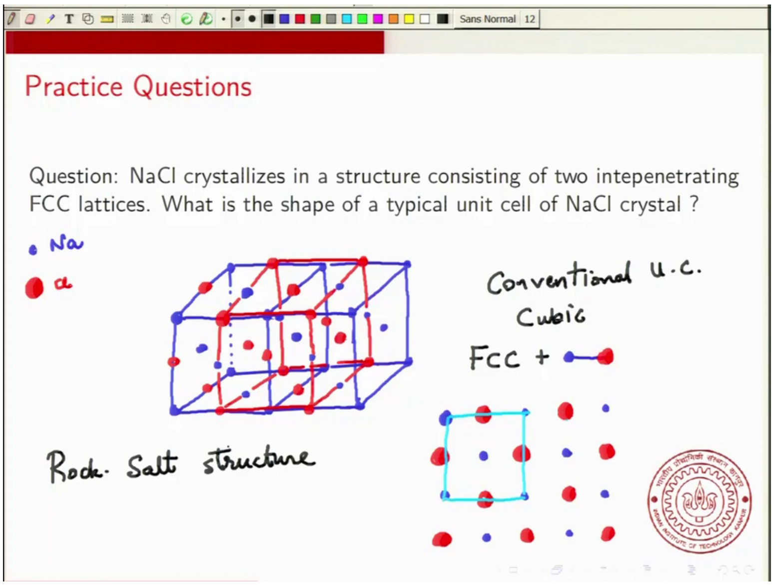

So, now, let us go to few questions, ok. So, there is a question. So, NaCl sodium chloride crystallizes in a structure consisting of two interpenetrating FCC lattices what is the shape of a typical cell of an NaCl crystal, and we want to identify the typical unit cell? Now, it turns out that NaCl has two FCC. So, let me and in particular this NaCl cell has a FCC formed by let me show blue for sodium and red for chlorine, for chloride and it is a classical ionic crystal, here which is so, the sodium ions form an FCC. So, this is the FCC formed by FCC lattice formed of sodium atoms, ok.

And now the chloride ions, they also form an FCC lattice, but now the lattice is actually shifted with respect to the sodium chloride, with respect to the sodium lattice. So, if I just extend this, I will just extend this in this direction just for convenience, ok.

And now, let me put the chloride ions. So, here you have a chloride ion here you have a chloride ion and you imagine making an FCC lattice with these chloride ions, ok. Now, these are right at the center of this of this edge, so at the edge center here you know, ok. So, this is the corners of, and additionally you have also at this edge center, this edge center, ok. So, what you can see is that if I just complete this then it will become very clear and there will be one on the rare face, one and one on this face, ok.

So, you can see that the chloride ions also have also formed an FCC, ok. So, both sodium and chloride are FCC and they are interpenetrating with each other. So, this is what your sodium chloride crystal looks like, and you can you can construct a unit cell, like so the typical unit cell, so the conventional unit cell unit cell is cubic, ok. Now, there are a few choices on how exactly to take your unit cell, you could either take a cube formed by, you can take this cube formed b; so, if we think of this as FCC plus a basis consisting of these two consisting of one sodium and one sodium and one chloride, ok.

The chloride is halfway along the along the lattice h, and you can see that this will generate the entire sodium chloride crystal, ok. So, I should also mention that there will be a chloride here, chloride here and so on. So, at each edge center there will be a chloride. So, essentially along any direction you will see an alternation of sodium chloride sodium chloride and so, sodium chloride and so on. So, this FCC with this 2-atom basis will actually generate the crystal, ok.

Now, if you just look locally what it looks like, it looks like you have sodium, let me show the sodium this way and you have your chlorides and I did not add.; so, few more sodium that also. So, if you look on any face, if you look at one, if you look at one face of this crystal then you will see something like this, ok.

And what this tells you is that you can find other unit cells, for example, this immediately indicates that you could take a unit cell like this such a cell, so that looks, so one more here. So, one choice of units also two choices of unit cell. So, one would be one would be something like this. So, that would correspond to this FCC with a 2-atom basis. We should be little more careful it will not be it will actually be just actually this is what will correspond to an FCC whether 2-atom basis, ok. So, this will be an FCC with a 2-atom basis, and so you can see that both the blue dots are in FCC and the red dots are also in FCC, ok.

Now, you can see that there is there is another way to do this, ok. So, just as you could also take these 4 as a part of the unit cell and again you could construct a suitable cell using that, ok. So, this is the structure of NaCl. So, the sodium chloride structure is one of the most common structures and it is it is seen in several compounds not just sodium chloride, ok. And this is it has a name this is called the rock salt structure, then we will see this as we go on in the course.

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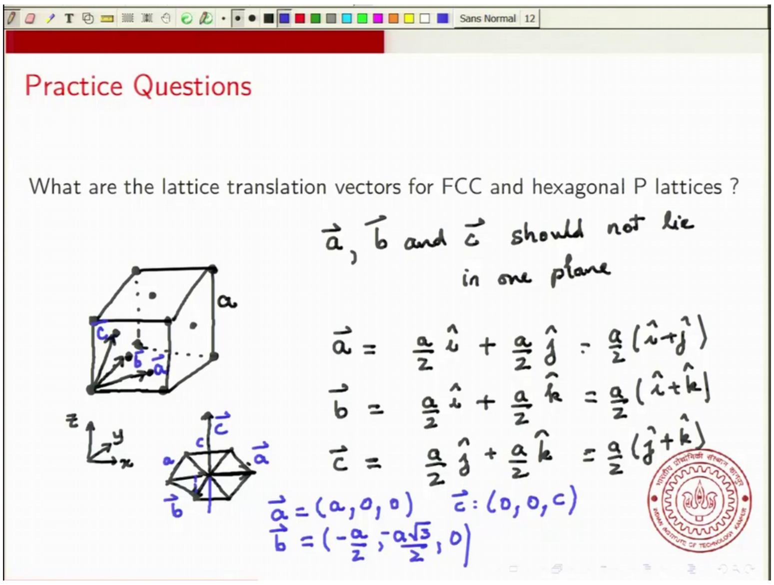

So, now, let us look at another question. So, what are the lattice translation vectors for FCC and hexagonal P lattices, ok. Now if you; so for an FCC lattice, ok.

So, you need translation vectors that will generate all the points, ok. So, one choice would be; so, your a, b and c should not all be in one plane, because if they are lie in one plane then any then their linear combinations will only give other points that lie in the same plane, ok. So, one choice I can show you. So, you can take for example, you can start from one corner and go to the 3 face centers nearest neighbor face centers, ok. And so, if you have if you have the 3 coordinate axis defined as let us say x, y, z, then the lattice translation vector a, if this is a and use a slightly different color. So, I will call this a, b and c, then a is equal to is equal to a by 2 where is this little a without the vector sign is the side of the square a by 2 i plus a by 2 j b is equal to in this case you have a by 2 i.

So, b is on the front face of this cube. So, it is a by 2 i plus a by 2 k and c is a by 2 j plus a by 2 k, ok. And you can see that if you take these 3 you will get, you will get a unit cell that is very that does not look like the conventional cell of FCC, ok. So, you can, I can write this as a by 2 i plus j, i plus k and this is a by 2 j plus k, ok. Now, you do not have to, I mean this is not you are not bound to take this choice you can also take other choices, because you just have to take 3 vectors that that do not line a plane and it they can be lattice translation vector. So, this is for the FCC lattice.

Now, for the hexagonal P lattice; so, the hexagonal P lattice is, in this case what you will do is you will have this. So, in this case we already saw that the cell can be described in terms of in terms of these two vectors. So, a, b and the c, c is in the in the third plane. So, c is in this plane that goes to the that goes to the other edge of the hexagonal cell, ok. So, these would be the primitive translation vectors.

And in this case if you express a as in this case if you say a is equal to and let me define this side as a and this, the other direction as c. So, a is and if I use the same coordinate system; so a is a, 0, 0 and your c vector is 0, 0, c; c is the is the distance to the next layer. But what about the b vector? Now, if you want to calculate what this P vector is, so, you see that it has a component on the x direction that is that is equal to minus a by 2. You have to you have to do some trigonometry, so if you drop a perpendicular here, then this length is a root 3 by 2 and this is minus it is a by 2 and it is in the negative x axis, so its minus a by 2. And then from the b direction is along the y direction is minus a root 3 by 2, and 0 along the z, along the z direction.

So, if you use this a, b, c, these are the a, b, c and Cartesian coordinates. So, these are in Cartesian coordinates, so I can write a as little a times i, c as little c times k, b as minus a by 2 i minus a root 3 by 2 j plus 0 k, ok. So, again this is not the only choice, you can also take other choices as its convenient, ok. So, this is how you get primitive lattice translation vectors for different lattices.

So, with that I will conclude week 2 of this course and we will start week 3 in the next lecture.

Thank you.