Introduction to Materials Science and Engineering
Prof. Rajesh Prasad
Department of Applied Mechanics
Indian Institute of Technology, Delhi

Lecture - 9
A symmetry based approach to Bravais lattices

Hello and welcome, this is going to be a very, very important lecture because we will with this lecture we will conclude our symmetry based approach to Bravais Lattices.

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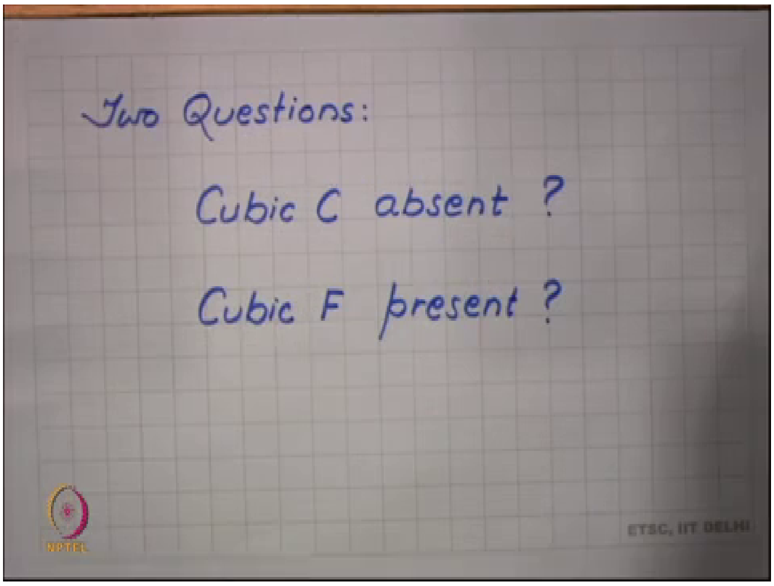

Recall, that we had 2 questions, why cubic C was absent in from the Bravais list? And why cubic F was present? We try to answer both these questions before we started with the symmetry based approach, but then we faced some difficulty and this was a difficulty, which forced us to take the symmetry based approach.

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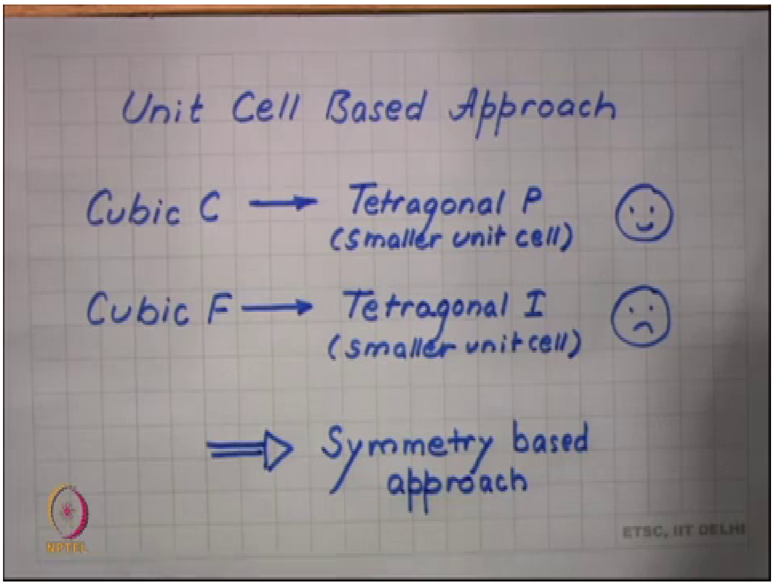

So, let us first recall what we got from the unit cell based approach. We found in cubic C by looking carefully, we found that we can select a tetragonal P unit cell and since this unit cell was a smaller, this was a smaller unit cell. We concluded that the tetragonal P was a better description for cubic C. So, we felt very happy, but then when we applied the same approach to cubic F we found that even for cubic F a smaller unit cell was possible and that was tetragonal I, the body centred tetragonal; simple tetragonal and body centred tetragonal.

So, face for face centred cubic; cubic F we can select a smaller unit cell which is tetragonal I, then why? Why not by the same argument tetragonal I is a better description for cubic F, if so we will reduce the number of Bravais lattices by 1 and will be left only with 13 Bravais lattices. This was a little disturbing and we were not very happy with this conclusion.

So, finally, this difficulty was what prompted us to look at the symmetry based approach, so this led us to the symmetry based approach and in the previous; several previous lectures we were developing the idea for or and concepts of symmetry. So, now, let us look at both of these questions from our symmetry based approach.

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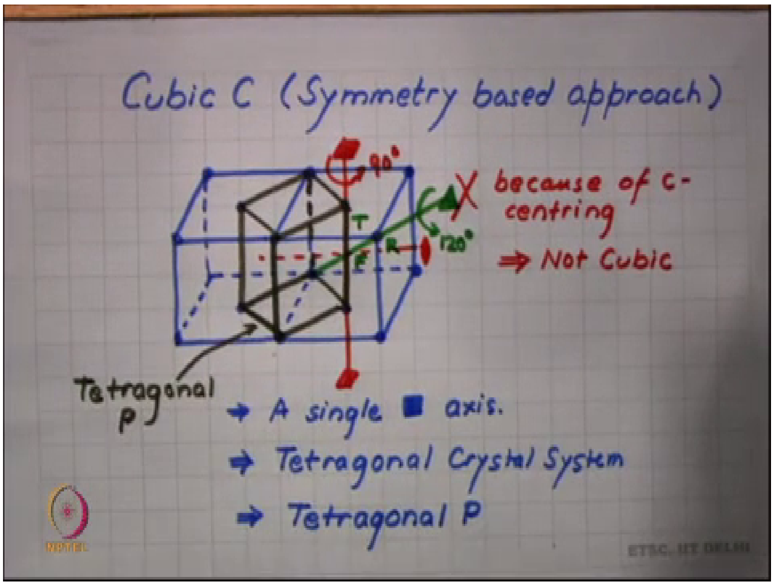

Let us first look at cubic C from the symmetry based approach. So, this is a cubic unit cell I place lattice points at the corners to make it primitive, but since I want cubic C, I place the top and bottom face centres also as lattice points.

Now, if we look from symmetry based approach, if we look, we should find out whether the lattice is still cubic. So, for cubicity or for the lattice to be cubic, we should look for the 3 fold axis along the body diagonal. So, let me draw 1 body diagonal this one is easier for me to draw, although anybody diagonal will do and this body diagonal I should examine whether it is a threefold or not. Recall, that threefold along the body diagonal, which involves a 120 degree rotation, exchanges the top face to the front face and the front face to the right face, the 3 faces are meeting and they go cyclically as I will rotate about this threefold axis.

So, if I rotate by 120 degree and if the top face comes to front face, in this case when we have centred only the top face and not the front face it is not a self coincidence, it is not a symmetry rotation anymore. So, because of the centring the threefold is lost, this threefold is lost because of centring; because of C centring, which leads to the conclusion that it is not cubic.

So, if it is not cubic there is no question of whether it is cubic C or not. So, the symmetry dictates that this lattice whatever it is cannot be a cubic lattice, then what it is? It is lattice of course, so what it is? To look for that again we look at symmetry, that what symmetry the threefold axis along the body diagonal is not there, but what symmetry is there. So, if you look at that, then you find that this vertical axis is preserved as a fourfold axis because faces are square and the lattice point is at the centre.

So, we can rotate by 90 degree about this axis to get our fourfold symmetry, are there other fourfolds? No, because the horizontal axis for example, because of the top and bottom centring and but no centring on the front face I cannot rotate by 90 degrees. So, this has become a twofold. So, only 1 unique fourfold is there in this lattice and we know. So, this is a, this is implying a single fourfold axis; a single fourfold axis is characteristic of a tetragonal crystal system.

So, the crystal system is tetragonal, so Bravais lattice also should be 1 of the tetragonal Bravais lattice, should either be tetragonal P or tetragonal I, simple tetragonal or body centred tetragonal because these are the only 2 listed in the Bravais list. So, to find that out which 1 it belongs to within tetragonal class, I add 1 more unit cell to look at symmetry often you have to draw more unit cells, we have been doing this now.

So, I add 1 more unit cell, again lattice points at the corner and lattice point at the top and bottom centres. If I do that, then I find that yes, indeed a simpler and a smaller tetragonal unit cell is possible if I join the lattice points in this way. So, this unit cell becomes tetragonal P, so the Bravais lattice we identify as tetragonal P. We came to the same conclusion by symmetry based approach, but now we have, we are standing on firm ground, we have good scientific basis or symmetry basis to claim as tetragonal P, our previous success in claiming it has tetragonal P simply by looking at unit cell wall just accidental or coincidental. So, the symmetry based approach is what we should look at.

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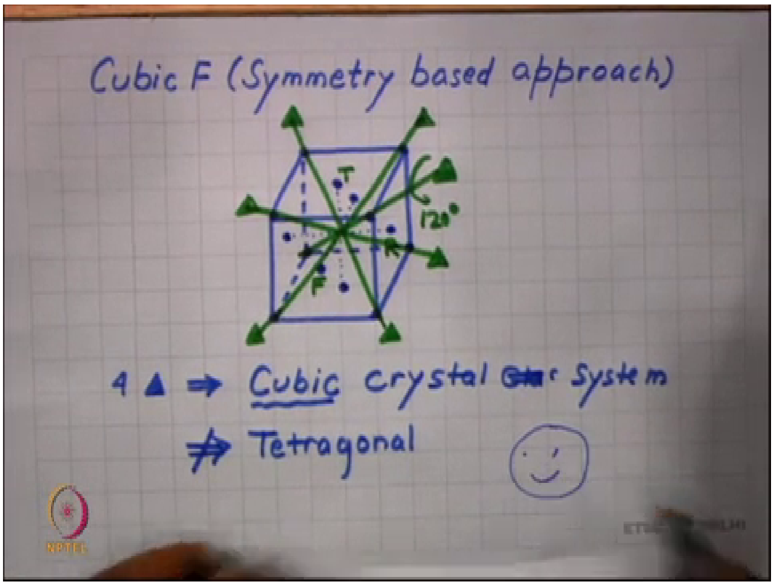

So, we continue with our second question, the presence of cubic F, which also in the unit cell based approach we saw that could be reduced to tetragonal I, but again the question is whether the lattice which has formed, the lattice with lattice points at corners of the cube and centres of all the faces front and back top and bottom and left and right is this, a cubic does this fall into cubic symmetry or does it fall into tetragonal symmetry.

Again, we start looking at our body diagonal and if we find, if we look at it because we have now centred the top face, the front face as well as the right face because of this centring when I rotate by 120 degree about this a centred top face will come at the place of a centred front face and the centred front face will move to the centred right face. So, each time, the cube and the entire lattice will come into self coincidence by this rotation, so the threefold symmetry does exist.

I have analysed for this threefold of course, you can do for other 3 folds also by symmetry all of them will have, for all the 4 threefold are preserved. So, since the 3 folds are preserved along the body diagonal, the presence of 4 threefold implies that it is cubic and we already have a nice cubic F unit cell. So, we do not go for a smaller volume unit cell which is tetragonal because the symmetry dictates that it is cubic; cubic crystal system and we will not take this into tetragonal. So, we have been saved, we have been able to save our cubic F face centred cubic from deletion from the Bravais list, which the unit cell approach was tending to do, so we are now happy.

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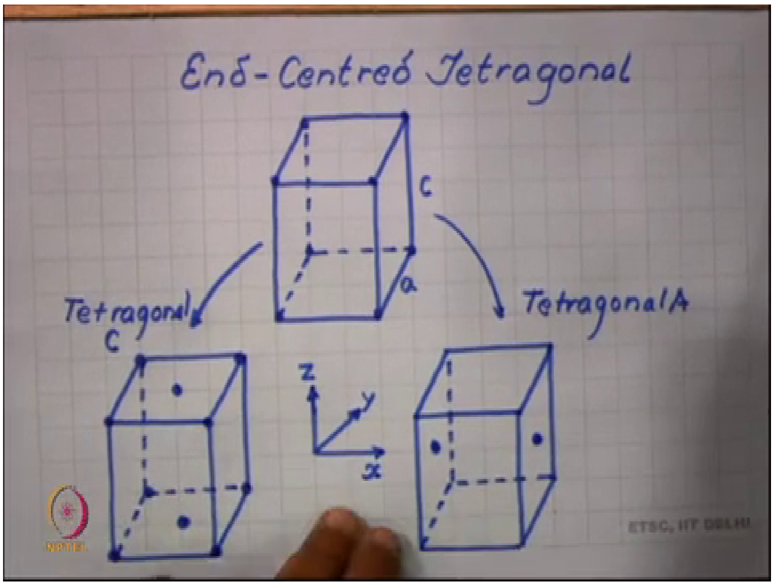

Let us look at 1 more example before we close our discussion on symmetry based approach, we take the end centred tetragonal. So, we start with the primitive end centred tetragonal sorry, we start with the primitive tetragonal and then we make it end centred by centring a pair of faces because the c axis is not equal to the, a axis. So, the top and bottom faces are square, where the side faces are all rectangle.

So, there are 2 ways in which it can be made into end centre either I can centre the top and bottom faces, that is the square faces or I can centre 1 of the side faces this will be since z axis is vertical, so this is the c direction, so this will be tetragonal C and this will be tetragonal A, but both are absent, there is no end centred tetragonal lattice listed in the Bravais list, why are they absent?

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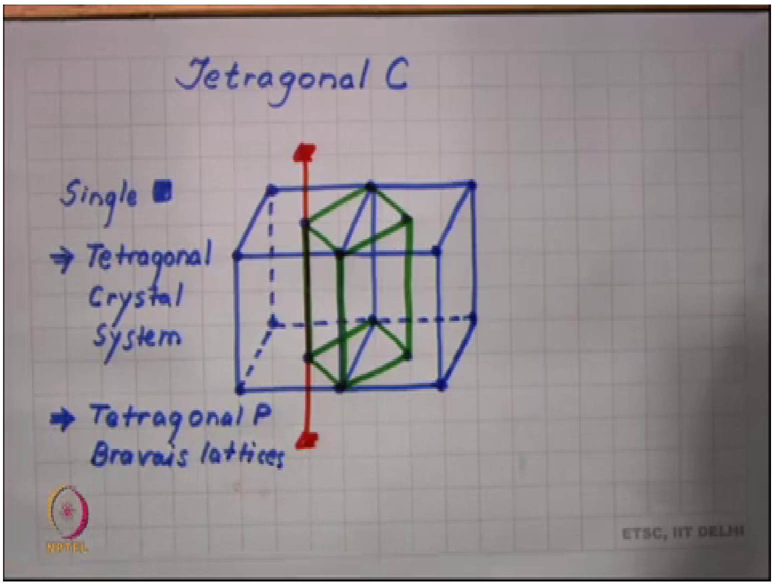

Let us again look at this question 1 by 1 from the symmetry approach. So, first we look at tetragonal C, if you look at the symmetry of this tetragonal C you can see that after centring since we are centring the square face, after centring this vertical fourfold which was the characteristic symmetry of tetragonal to begin with is preserved. So, single fourfold is preserved. So, we conclude that yes, indeed it is tetragonal, but if it is tetragonal, why this is not listed. So, we this indicates that there must be different choice of unit cell available indicating that this is a different Bravais lattice.

So, we again do that by our familiar trick which we have now used many times, we add another unit cell, add the centring points and just carve out a simpler and a smaller tetragonal P Bravais lattice. So, 1 fourfold said that it was tetragonal crystal system, but in the tetragonal crystal system there is no tetragonal C. So, by our new choice of unit cell we are able to identify it as tetragonal P Bravais lattices, this explains away tetragonal C, that why tetragonal C is absent.

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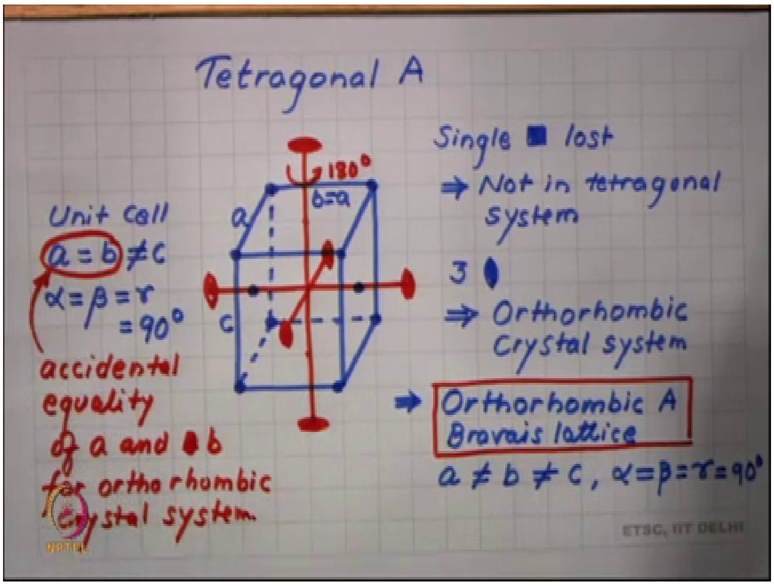

But, the tetragonal A makes a more interesting case, so let us look at here, tetragonal A case. So, they of lattice point at the corners and then 1 pair of rectangular faces now. As soon as you centre the rectangular face, you can see that you have lost the fourfold character of the vertical axis, the vertical axis is no more to fourfold because if I rotate by 90 degree, this left face will come to the front where there is no centring.

So, it is not the lattice is not mapped into itself, but if I rotate by 180 degree, the left and right faces will exchange and everything will come into self coincidence. So, this axis instead of being fourfold becomes twofold. So, since fourfold is lost, it is no more tetragonal, single fourfold lost due to centring who not in tetragonal system. A single twofold is characteristic of which crystal system? This is the characteristic of monoclinic system, so is it monoclinic? Well, we have to be little bit more careful in jumping to that conclusion because we have not analyzed all the symmetry.

Let us look at the symmetry along x and y axis, along this axis. So, we find that along this axis, also if we rotate by 180 degree because this face is a rectangle, rectangle will come into self coincidence by rotation of 180 degree, this is also a twofold and the third axis also is twofold. So, by symmetry it had 3 mutually orthogonal 2 folds, this indicates that this is orthorhombic. If it is orthorhombic, there is no problem of end centring because end centred orthorhombic is an acceptable Bravais lattice.

So, it is orthorhombic crystal system and within that crystal system we have orthorhombic A Bravais lattice no problem, but there is 1 problem and the problem is again of the unit cell shape. If we focus at the unit cell shape, the unit cell it is satisfying a equal b, these sides being a square are equal.

But not equal to c as the third side and all 3 angles alpha, beta and gamma are of course, 90 degree, but this unit cell shape is characteristic of a tetragonal unit cell, but by symmetry we are coming to the conclusion that is orthorhombic A Bravais lattice, by unit cell shape it seems to be indicating tetragonal, what shall we do and the orthorhombic unit cell demanded a not equal b, not equals C, alpha, beta, gamma equal to 90 degree. Well, there is no problem, we will give symmetry the priority and based on symmetry we will call it orthorhombic A Bravais lattice.

And, it is so, happens that in this case the unit cell a equal b, we will simply accept that had accidental equality; accidental equality of a and b sorry, a and b or orthorhombic crystal system. So, although, so this is very, very good example that although the unit cell shape is tetragonal, but symmetry is orthorhombic I will still call it orthorhombic A and equality of a and b will be taken as accidental equality. With this, we end our journey of symmetry a through Bravais lattice and we will now, close this chapter and in the next session we will take up the specification of directions and planes in crystal through miller indices.