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

Lecture - 05 Gaps in Bravais lattice list

In the last video we saw the list of 7 crystal systems and 14 Bravais lattices.

(Refer Slide Time: 00:14)

I	Cubic	P	I	F	X
2	Tetragonal	P	I	C. I.	
3	Orthorhombic	P	I	F	C
4	Hexagonal	P			
5	Trigonal	P	7.468		
6	Monoclinic	P			C
7	Triclinic	P	1000		1000

Here is the less we have 7 crystal systems cubic Tetragonal, Orthorhombic, Hexagonal Trigonal, Monoclinic and Triclinic and we have 14 Bravais lattices represented by these symbols. Recall that P is stands for primitive, which means lattice points are only at the corners of the unit cell, I is stands for body centred, where lattice points are at corners as well as at the centre of the unit cell, F is stands for face cantered where we have lattice points at corners as well as all the 6 face centres of the unit cell.

And finally, C is stands for base centred or end cantered where the lattice points are at corners and centres of only 2 parallel faces of the unit cell. We ended the last video with a central question of why there are. So, many empty boxes in the Bravais list in particular why do not we have cubic C, this question is central to the understanding of this list.

So, let us write down that question why cubic C or end cantered cubic end cantered cubic is absent from the Bravais list answering this question will lead us to in interesting conclusion about the basis of classification of these lattices.



(Refer Slide Time: 02:20).

So, let us look at what do we mean by End-cantered cubic lattice; End-centred cubic lattice. So, here is a cube I put points at the corners and I also put points at 2 parallel faces of the unit cell I select the top and bottom faces. So, if I repeat this unit cell I will generate a set of points, which I would like to call the end cantered cubic lattice. The question is why is it not there in the list is it not a lattice let us explore first whether by at adding these additional points we still have a lattice this question can be better answered if we look at a few more unit cells.

So, let me add a few more unit cells I am just starting cubes next to the cubes which we were having in the beginning resulting in a 2 by 24 unit cells with one common vertical edge and if I add the points where they are expected to be. So, that is the corners and the top and bottom faces top and bottom face the diagram is really getting a little complicated, but you can imagine what we have drawn we have drawn 2 by 2 4 unit cells each of them have points at the corners as well as point at the centres of the top and bottom faces.

Now, if I shift except the origin instead of drawing my corner there supposes these centring points themselves I take as my corners. Then you can see that the role of centres

and corners have changed in this new unit cell, what was corner of the original cell is now the end centre of this new cell and what was the end centering points of the original cell is the corners of the new cell.

So, this shows that these the new points which we have added the End centring points are equivalent to the original point. So, they do form a lattice. So, we do have an End centred cubic lattice is not a mistake in that sense it is a lattice all points are equivalent translational equivalent to form a lattice then why it is not in the list.

Let us look at this once more.



(Refer Slide Time: 06:39)

Let us create again 2 end centred cubic lattices side by side. So, they have a common face in between. So, 2 cubes with a common face and if they are unit cells of the end centred cubic and I put points lattice points at the corners, now we are convinced that all points are lattice points lattice points at corners as well as lattice point at the face centres, but only one pair of face centres. So, top and bottom face centre.

Now, with little imagination you can see that it is possible to select a new unit cell. Now I am outlining in red a possible new unit cell for the same lattice in red. So, this was this was the original end centred cubic unit cell and in red we have outlines a new cell a new unit cell what is this new unit cell what is the shape of this new unit cell. So, let us call this this side a prime this side b prime and the third side the vertical side is c prime.

So, we can quickly c that a prime and if I call this the original cube and a then a prime is half the face diagonal. So, face diagonal is root 2 a divided by 2. So, a prime is a by root 2.

Similarly, b prime is also the half the face diagonal. So, that is also a by root 2 whereas, c prime is equal to the cube edged is the vertical cube edge. So, c prime is just a so we see and if we look at the angles, angles are still all 90 degree. So, we have alpha beta gamma as 90 degrees. So, in this new unit cell we have a prime equal to b prime not equal to c prime alpha equal beta equal gamma 90 degree. This is a shape of a tetragonal unit cell this imply a tetragonal unit cell and if you look at the lattice points if you look at the lattice point you find that lattice points are only at the corners. So, this is a primitive Tetragonal.

So, which means what we have here is a Tetragonal P unit cell which brings us to now the question that we started with end-centred cubic unit cell we started with end centred cubic unit cell, but a different choice of unit cell we can describe the same lattice as primitive tetragonal or simple tetragonal.

So, what shall we call this lattice should we retain end centred cubic or should we retained should we call it tetragonal P Bravais; obviously, does not have end centred cubic, but he has tetragonal P. So, we can justify that this lattice is already as a tetragonal P in Bravais list. So, we do not need end centred cubic we can give a further justification by noting that the unit cell volume of the tetragonal P is a smaller tetragonal P has only half the volume of cubic c. So, it is a smaller. So, if I have a choice between end centred cubic and tetragonal P I can say that I will choose a smaller unit cell which represents the lattice if you accept this argument then you will run into problem soon.

(Refer Slide Time: 13:34)

Face-centred Cubic (Cubic F) For Cubic F - Tetragonal I + Tetragonal P

Let us look at face centred cubic lattice. So, we are now looking at face centred cubic or cubic F and I am again drawing to you in itself side by side 2 face centred cubic unit cell with one common face they are sharing this metal face. And since they are face centred cubic let me place the lattice points lattice points at all corners all the corners are lattice points as well as I have to put lattice points at the centres. So, centres of the top and bottom face centres of the left and right faces and centres of the front and back faces and if we apply the same procedure of identifying a new unit cell which we did for showing that cubic c reduces to tetragonal P, we identify an identical unit cell in the same process.

So, red unit cell is representing our new choice of unit cell in this lattice. And now if you look at the location of lattice points you have them at corners you have them at corners and you also have one in the body centre of this new unit cell, because what was at the common face centre is now become the body centre of this red unit cell.

So, which means even for face centred cubic we can select a tetragonal body centred unit cells. So, cubic F can be reduced to Tetragonal I, but then why Bravais has kept cubic F when we when we had cubic C yes Tetragonal P we deleted cubic C and we kept Tetragonal P, but now we are able to show that cubic F is tetragonal I, but we are still keeping cubic F as well as tetragonal I why is this. So, this is a very very important and deep question, which brings us to the basic definition or basic classification of crystal

systems and Bravais lattices if we can reduce cubic F to tetragonal I we will reduce the number of Bravais lattices to 13.

So, has Bravais over counted this kind of over counting is not unknown in history.

HISTORY 1835 M.L. Frankenheim 15 lattices 1848 A. Bravais 14 lattices 1856 M.L. Frankenheim 14 lattices

(Refer Slide Time: 18:21)

There has been an instance where in 1835 M L Frankenheim came up with 15 lattices apparently the over counted, perhaps he counted 3 monoclinic lattices instead of just 2. Then 13 years later Bravais identified this mistake and gave his corrected list of 14 lattices, without seen Bravais result Frankenheim 8 years later in 1856 also corrected his own mistake and came up with 14 lattices, but as you know now we call these lattices as Bravais lattices and not Frankenheim lattices because of his earlier mistake. So, history can be very hards sometimes and maybe the credit should have been shared between the 2 discoverers and the lattice could have been called a Frankenheim Bravais lattice.

So, let us put the conclusion of this video what we have concluded is that essentially the problem is that we are trying to classify lattices by looking at the unit cell shape.

(Refer Slide Time: 20:08).

Lattices CANNOT be classified on the basis of unit cell shapes. (: infinitely many unit cells are possible) What is the relo real basis for classification of lattices. SYMMETRY ETSC, IIT DEL

This will lead us inherently into problem because we know that a single lattice can be represented by many different unit cells. So, once we realize this that a single lattice can be represented by many different unit cells, we conclude that lattices cannot be classified on the basis of unit cell shape, because infinitely many unit cells are possible we have seen this are possible, but then the question is what is the basis for classification of the lattices what is the real basis for classification. The answer to this question is symmetry and we will look at the concept of symmetry and how it is used for this classification in the next and future videos.