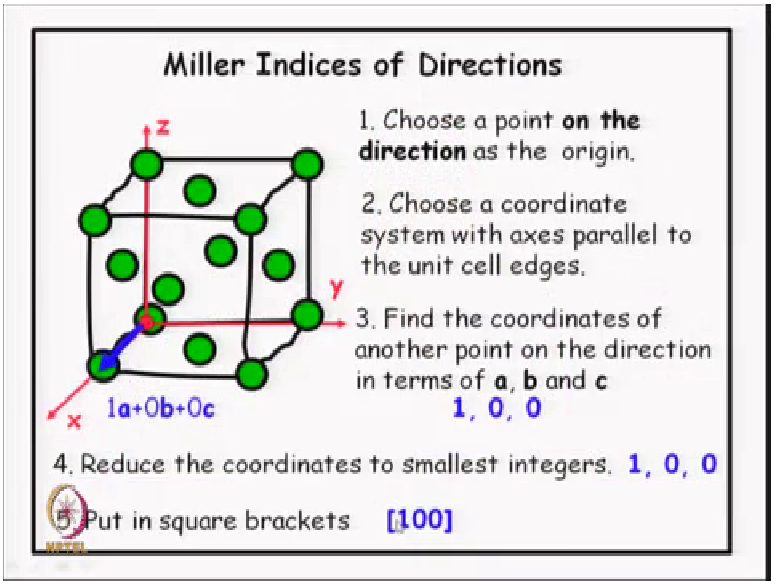
Introduction to Materials Science and Engineering
Prof. Rajesh Prasad
Department of Applied Mechanics
Indian Institute of Technology, Delhi

Lecture - 10
Miller indices of directions

Hello, today we will start a new topic till now; we have been discussing bravais lattices, 14 Bravais lattices and 7 crystal systems. We looked how symmetry helps in classification of crystals into these schemes. We will now start a new topic the miller indices of directions and planes. These are techniques or tools to specify a various directions as when we work with crystals, we need to specify or name different directions and planes in a crystal. Miller indexing is an standard method which has been which is being used for this purpose.

Let us look, we will first in this video we will look at miller indices of directions and in the next 1 we will take miller indices of planes.

(Refer Slide Time: 01:06)



Let us look at miller indices of direction suppose we have this crystal a unit cell is shown a face centred cubic lattice. All these large circle are the lattice points and we want to specify a certain direction. Let us say this blue direction edge of the cube now. Of course, the cube has this edge. It has this another edge 2 horizontal edges and 1 vertical edge. I have picked out 1 of them this blue 1 and I want to give a name to it. Of course, in common language I can say that it is the edge of the cube on it is bottom face coming out of the screen to say and this 1 is an edge lying in the screen and this is a vertical edge and so on; however, miller indexing will give us a specific notation, a specific system to name this blue line.

Let us look at how we do that we will go step by step. The first step in miller in indexing is to choose an origin on the direction. So, I have chosen this back corner as my origin, pointed out in red. So, the first step is always to choose the origin and I have highlighted here that on the direction. The origin always has to be on the direction it should lie on the direction or vice versa the direction should pass through the origin or origin should be so chosen that it lies on the direction.

This freedom of choice exists in crystallography in the crystallographic coordinate system; we are free to choose the origin anywhere we wish. If I want to index this blue direction I choose the origin on the blue direction and I took this point as the origin. The next step is to choose a coordinate system, crystallographic coordinate system with axis parallel to the unit cell edges. In this case I have chosen X, Y and Z with the 3 XYZ directions parallel to the unit cell edges here, I have red for illustration purpose, I have taken a cube even in a non cubic crystal even if the angle between X and Y is not 90 degree and even if Z is not perpendicular to X and Y we will always choose our X, Y and Z parallel to the unit cell edges, this is what is called the crystallographic coordinate system.

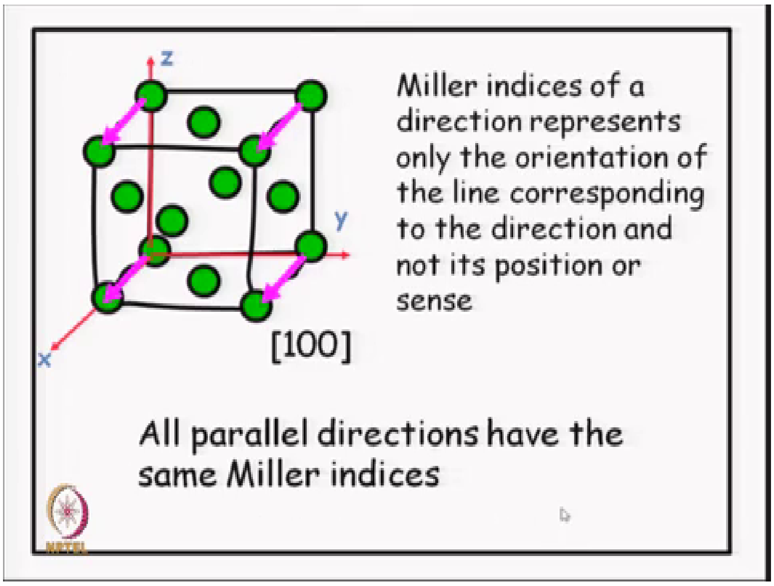
We will be using the crystallographic coordinate system with unit cell edges as our axis. We have d1 that for this direction, now we have taken this red origin and red axis the next step is to find the coordinates of another point on the direction in terms of a b and c a b and c are the 3 lattice parameters. In this case, they are the edge lengths a is the edge length of the unit cell along the X axis, b is the edge length of the unit cell along Y axis and c is the edge length along the Z axis.

So, in terms of these 3 vectors the a b and c vectors I i will now try to express the blue vector, which is the vector of my choice direction of my choice ad in terms of these 3 vectors. Here it is very simple it is 1 times a because the direction is along the X axis and it is of the length equal tO H. It is 1 times a 0 times b and 0 times c. I just take these coefficients 1 O O to represent this direction. So, I find the coordinates of another vector in terms of a b and c. So, the first 1 means 1 times a, the second 0 means 0 times b, and then 0 times c. The next step which in this case a redundant, but we will write it out because we will use it in the next example is to reduce the coordinates to smallest integers and this can be d1 either by dividing by a common factor or multiplying by common factor.

Suppose, we had fractions then, we will multiply by some common factor such that the fractions get cancelled or suppose if we had a common factor in all these 3 then we will divide by that common factor to cancel out the common factor. So, this is a step of reducing the coordinates to smallest integers in this case and nothing is required 1 0 0 is already smallest integers. So, we carry on with that and then the final step is to just put these 3 numbers in a square bracket there is an important step, a square bracket is not my choice in this presentation or this slide it is an internationally agreed upon convention the directions will always be represented by numbers inside square bracket. So, we will follow this convention. So, 1 0 0 is the direction which is represented by this blue line.

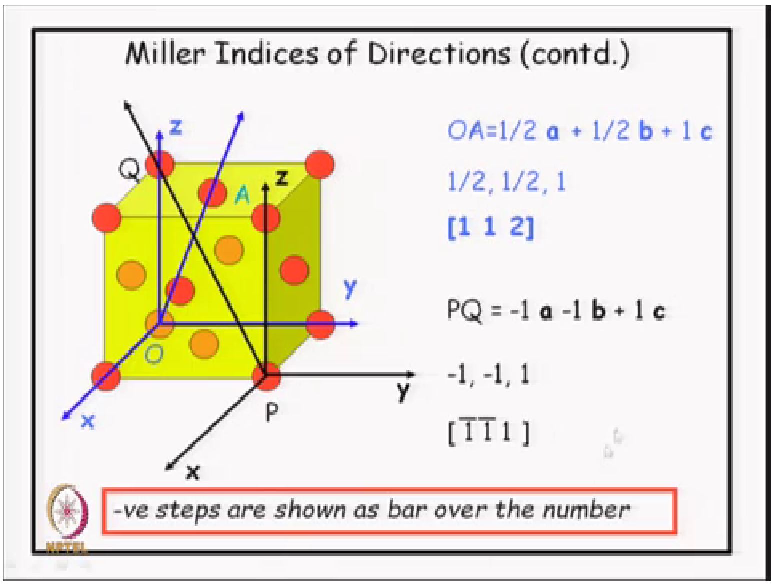
So, 1 0 0 there is a slide difference between vector terminology and the miller indices of a direction although I picked up 1 vector this blue vector toO Hlong this line and you use that to calculate my miller indice once I have found the miller indices 1 0 0 it is not representing just this blue vector, but this entire X axis. So, the entire X axis as well as the negative X axis can be represented this full line is represented by the number 1 0 0 another peculiarity of convention here when I wrote the comp1nts separately I am writing it with commas, but in the miller indices I am not using any commas. This is a useful convention unless and until we have a 2 digit miller indices for 1 of the comp1nt if, it is only 3 numbers we write them without any commas and it is understood that the first number is with respect to the X axis the second 1 with respect to the y and third 1 with respect to z.

(Refer Slide Time: 08:30)



Let us look at some more examples now, before looking at those examples 1 more point. Miller indices of a direction represents only the orientation of the line not it is particular position in space or also it is sense, I already told that not only the positive X axis, but the negative X axis will also be represented by 1 0 0 if we do not really want to distinguish positive and negative that is to say, if we are only interested in the line not in the sense and in miller indices that is usually the case then 1 0 0 represents the entire X axis not only that because what we said about freedom of choosing the origin, if we had parallel lines somewhere here then, I can again choose my origin here and this will become my X axis or I can choose my origin there and this will become my X axis. So, all parallel directions have the same miller indices.

(Refer Slide Time: 09:42)



Let us now look at some more examples. Again we take this face centred cubic unit cell and we want to indices a direction which is starting from this corner and passing through the top face centre. This direction is the direction of my choice. So, I choose this as a coordinate first step to choose a coordinate origin and a coordinate system. So, I chose this point as my origin and axis along the unit cell edges. With respect to this coordinate system I now write the vector O H. So, you can see to reach O H, I have to go H by 2 steps along XA by 2 steps along Y and then C step along Z. O H the vector O H is 1/2 a plus 1/2 B and 1 times C. So, the coordinates which we will use in the miller indices in terms of AB and C are ½ 1/2 and 1.

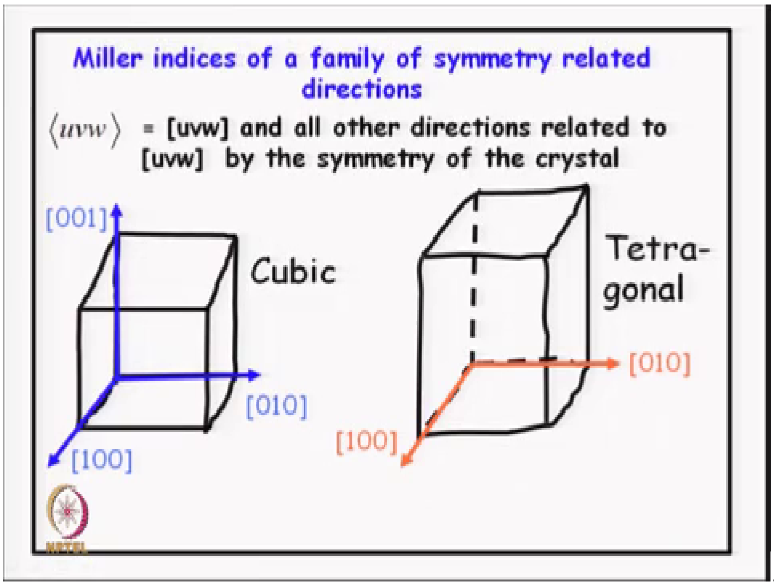
Now I will use the cancelling of fractions step which we did not require in the previous 1 in the case of 1 0 0 we did not require that, but now in the case of ½, ½, 1 we will not call this direction 1/2 ,1/2,1 but will simply multiply by 2 all these 3 numbers to get 1 1 2 and of course, I put them in the square bracket which we have agreed upon to use as a convention for directions. So, the O H direction not just the O H vector, but the entire O H direction will be represented by this miller indices 1 1 2 1 more example, let us look at this black direction now of course, I have to choose the origin on the black line and that freedom is there.

So, I shift the origin to this point P on the black line you can note that when I have shifted the origin, I have kept the axis parallel. So, we have the freedom to choose our origin anywhere, but in a given problem once we have specified the orientation of the axis the that orientation cannot change. So, the XYZ in the new with the new origin is exactly parallel to the XYZ before the black XYZ is parallel to the blue XYZ. Now, let us try to indices this direction along PQ which is 1 of the body diagonals of this Q. So, if we want to look at this PQ we will start with p and you can see that now I have to take a minus 1 step along X 1 step along Y and 1 step along Z to reach Q. So, the PQ vector is minus 1 a minus 1 b and 1 c.

So, the components are minus 1 minus 1 1 in terms of a b and c now I write this in a square bracket with 1 additional convention that the negatives are written as bars over the number instead of on the side as in useful mathematics in the miller indice indexing notation, a bar above the number represents negative quantity. So, and it is red also has bar instead of minus 1. So, we will call this direction PQ as my bar 1 bar 1 1.

Let us now take. So, the negative steps are shown as bar over the number.

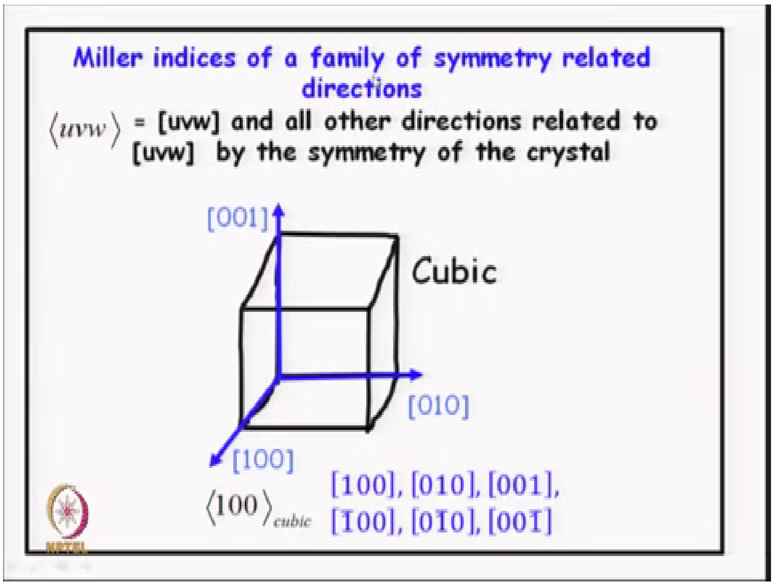
(Refer Slide Time: 14:04)



Let us now look at another convention which is used many times, we are not interested in just 1 direction because we have talked about the symmetry in the crystal and crystals can have symmetry and symmetry relates many directions. So many directions become equivalent because of the existing symmetry of the crystal. For example, if you take a cubic crystal, all the edges of the cube are equivalent by the cubic symmetry. If we if we indices the edge along X axis it will be 1 0 0 if we indices along the Y axis 0 1 0 and indices along Z axis 0 0 1. But suppose I am not interested in a specific direction, I just want to talk about the cube edges for all directions along the cube edge which are equivalent by symmetry.

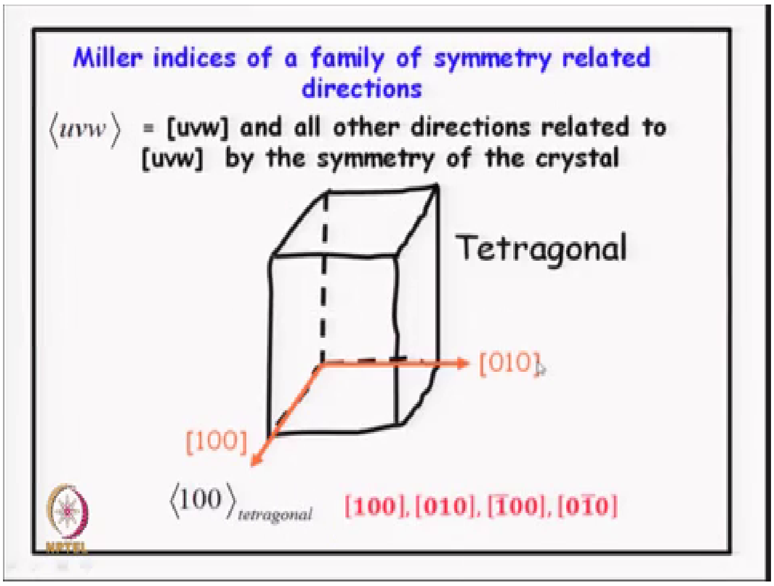
Then there is a new notation that you can put the miller indices of any 1 of them in an angular bracket. An angular bracket u v w means the specific direction u v w and all other direction related to u v w by the symmetry of the crystal. And it is important that when we are using this notation we have to know which crystal system we are talking about because different crystals will have different symmetry and the symbol will mean different things. We will show you this with the help of cubic and tetragonal examples.

(Refer Slide Time: 15:49)



So, let us look at first the cubic, in the miller indices of cubic crystal the 1 0 0 direction is equivalent to 0 1 0, 0 0 1 as well as if you take the negatives minus bar 1 0 0, 0 bar 1 0 and 0 0 bar 1. So, the all 6 direction are equivalent by the cubic symmetry. So, if we simply write 1 0 0, if I pick any 1 of them I have picked up 1 0 0 you could have picked up 0 1 0 or 0 0 1 any of these 6. So, any member of this direction this is a family of 6 members, this is a family of symmetry related directions and I pick up any member of the family to represent the entire family. So, when I say 1 0 0 in angular bracket and I know that it is for cubic then ill mean all these 6 directions, but now.

(Refer Slide Time: 16:56)



Let us look at the tetragonal crystals in tetragonal you know X and Y are equivalent by symmetry, but not the Z. So, if I say 1 0 0 for tetragonal, it will only mean these 4 directions 1 0 0 0 1 0 and their negative the third direction, 0 0 1 is absent from here in this list because tetragonal symmetry does not make 0 0 1 equivalent to 1 0 0.

With this, we will end this video. In the next video, we will take the discussion on miller indices of planes.