Crystals, Symmetry and Tensors Professor Rajesh Prasad Department of Materials Science and Engineering Indian Institute of Technology, Delhi Lecture 2b Miller Indices for Directions

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Now the Miller indices, another important concept. So, Miller indices is there for direction as well as planes. So, let us first discuss direction, Miller indices of direction. So, AB is a direction AB is a direction again I have taken that same unit cell, the sodium chloride unit cell. So, just as an example and I am thinking of a direction A to B. For defining the Miller indices, two important things are there, first, where you will choose the origin, you have to choose an origin and x y and z.

One thing is defined that because we have to work in crystallographic coordinate system and axes of the crystallographic coordinate system has to be parallel to the edges of the unit cell that we have seen. The unit cell and origin at a corner which is a lattice point however, still there is a lot of degrees of freedom left for me. First of all, this unit cell has 8 corners. So, I can choose any of the 8 corners as my origin.

And then from each corner, 3 edges of the unit cell emerge, 3 edges of unit cell me at each corner, which one I call x, y and z is again my choice what I am calling x, you may be calling y and we may fight unnecessarily. So, we have to be very, very clear, there should be a clarity of which corner we have selected as the unit cell and which edges we are calling x, y and z.

So, for Miller indices of direction one of the convenient although not necessary, but one of the convenient choice of origin is to choose the origin on the direction itself. At one point of the direction. So, for A B, I will choose the origin at A and then for this problem, we have once for all decided that my x axis will be pointing this way, y axis will be pointing this way and z axis will be pointing this way, as shown here on the side.

Since the freedom for choosing the origin was there, that is why I showed the axis away from the unit cell and not embedded on the unit cell. Because I do not want to give preference to any corner wherever I draw this on any corner so that top corner becomes a special chosen origin the chosen one, but I do not want to initially give that status of the chosen one to any. So, when I come to figure out AB direction, then I choose A as origin.

So, if I choose a as origin and then my direction AB is along A. So, the vector a is 1, o, o. It is a, o, o if you want but we have already defined the fractional coordinate. So, we will divide by A. So that becomes 1, o, o. The components of the vector components of the vector in the direction itself is the Miller indices. So, we have found the Miller indices of AB. So, this is the Miller indices of AB it is just a vector.

Although it is a vector, when we say it is Miller indices of direction, we imagine that we are talking about this entire direction. Vector a has a fixed length, so, I could have chosen any vector along this length. But I will get the same miller indices, how if I choose twice the vector, then that will become 2, 0, 0. So, I introduced one more step in deciding the Miller indices, that if you can divide by a common number, you are allowed to do.

So, divide by some common number to reduce it to smallest numbers. So as soon as I see 2, 0, 0 I divide by 2 to get 1, 0, 0. So even if I had selected a longer vector, or if I had selected a shorter vector, half, 0, 0, then I will, I am allowed to multiply by some common number to get 1, 0, 0. So, 1, 0, 0, half, 0, 0 and 2, 0, 0.

In terms of vector, if we are thinking in terms of vector and sometimes you want to think in terms of vector, so there is nothing wrong, then there are three different vectors all in the same direction, but of different length. But if I am thinking in terms of Miller indices, I will reduce all of them to 1, 0, 0 and say, I am talking about the 1, 0, 0 direction. So, 1, 0, 0 direction will always be the x direction will always be the direction along the a of your unit cell.

So, let us now look at some other direction AG, AG direction. So, what will you get? Yeah? AG? Yeah? 1, 1, 0, one along a, one along b. So, essentially the in terms of vector. So, see, if I write it as a vector AG, so I will write 1 times a plus 1 times b plus 0 times c. So that is the vector in terms of coordinate it becomes a, b and 0, in terms of coordinate. But then in Miller indices, we use the fractional coordinate.

So we will divide first one by a second one by b and third one by C. So I get 1, 1, 0. You can see while we are calling it 1, 1, 0. The two 1s are not equivalent, the second 1 is representing a length b. Here in NaCl unit cell since it is cubic A and B lengthwise also are equal but even if they were unequal, this face diagonal direction will always be 1, 1, 0. But the second 1 will be representing B step of a different length and the first 1 a step which one we should do now?

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GF, what is GF?
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Student: (())(9:48)

Professor: So, what is your chosen origin now? It is nice to choose the origin here now. We were working with a because we were having AB and AD. But now we have GF, so we shift, we bring our origin here. And if we bring our origin here and choose, when you shift in one problem, initially, you are free to choose your x, y and z also, I told you which one you call x, which one we call y, you are free.

But if I am doing one exercise one problem, then once chosen, the x, y, z orientation, when I shift the origin for my convenience, I do not flip the x, y, z. So, x, y, z I have to keep the same. So, then I have to from going from A to F, I have to go minus 1 along x minus 1 along y and 1 along z. So minus 1, minus 1, 1 and in crystallographers decide to write minus on the top as bar. So that is the Miller indices of direction