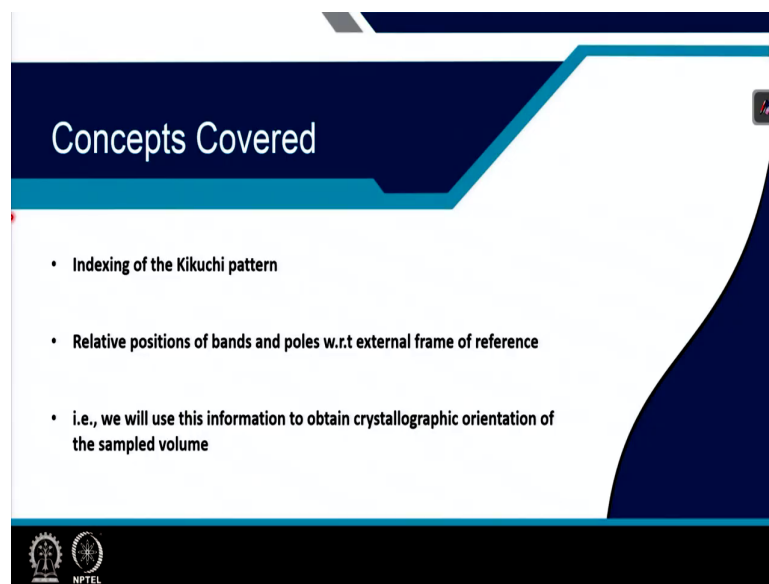


Texture in Materials
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Module - 06
Microtexture measurements using EBSD technique in SEM
Lecture - 32
Quantitative Evaluation of Kikuchi Diffraction Pattern - I

Good afternoon everyone and we are continuing with the module 6 that is Microtexture measurement using EBSD techniques in SEM. So, this is lecture number 32 and this is regarding how we will quantitatively evaluate the Kikuchi diffraction pattern; the name of the lecture is Quantitative Evaluation of Kikuchi Diffraction Pattern. So, this is part 1.

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The concepts that will be covered in this lecture are indexing of the Kikuchi pattern; relative positions of bands and poles with respect to the external you know frame of reference that is sample frame of reference and that is we will use the information to obtain crystallographic orientation of the sampled volume.

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o Zone axes - Axis-12, 23, 31.
 $\alpha_{12}, \alpha_{23}, \alpha_{31}$

o ND/BN \rightarrow incident e⁻ beam direction.

o RD \rightarrow - rotating the sample in TEM kept in copper grid

o RD \rightarrow from a single Kikuchi pattern

$n\lambda = 2d\theta$
 $2\theta = \frac{n\lambda}{2d_{hkl}}$

So, we will do this by using the you know Kikuchi pattern and example Kikuchi pattern from the book of Valerie Randle and Olaf Engler. And you can see that the bands are you know forming and we have given for example, the band 1, the band 2 and the band 3 right. The All these bands, the hkl planes will have to calculated from the you know distance between these two lines of a particular band.

And say for example, if this is 2 theta b 1 and this is 2 theta b 2 and this is 2 theta b 3. Then, if we have calibrated the distance between the sample and the phosphor screen, then this distance in length of these bands could be calibrated and then, we can know the two thetas of these bands right.

Thereby, once we know the 2 thetas of this band, then by using the formula n lambda is equal to 2 d theta which is true for the electron beam with a very low wavelength. Of course, those are of very low wavelength. One can relate this theta or 2 theta b with respect to you know n lambda by 2 d of that particular h k l and therefore, we can find out the value of h k l right.

So, if we can find out the value of this band which is h 1 k 1 l 1 and this is 3 bar 1 1 and if this is h 2 k 2 l 2 as 2 2 bar 0 band 3 as 0 2 2 bar. Then, you see we can calculate the zone axis. So, the first thing is that we will calculate we will see how mathematically we can obtain the zone axes right; the three zone axis that is axis 12, 23 and 31.

Secondly, if we can know the angle between the 2 lines of a band 2θ , then if the distance of the sample and the phosphor screen is well calibrated, then we can also find out the angle from the pattern center to these zone axes right.

So, if we can find out what is α_{12} , α_{23} and α_{31} from the Kikuchi pattern, we can relate this to find out the value of ND which is also known as beam normal or the incident beam electron beam direction right and then so, this is the one thing, we will find out; this is the second thing, we will found out.

And then, we will try to found out RD in terms of Miller indices of the sample by rotating the you know sample in a TEM kept in sample which is kept in copper grid. And we will also try to find out RD from a single Kikuchi pattern that is a single whole, this whole Kikuchi pattern right. So, let us go ahead.

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• $NP = ON \tan(\tau) \rightarrow \tau$ is the angular displacement of P from the pattern centre N

$NP = ON \tan(\tau) \approx ON(\tau)$

Assumption:

The diffraction pattern though gnomonic projection, the distances near the pattern centre (N) can be considered to be scattered linearly with the projection angle τ

The diagram shows a sphere with a flat phosphor screen. A point O is at the center of the sphere. A point N is on the surface of the sphere. A point P is on the flat phosphor screen. A line ON is drawn from the center to the point N . A line NP is drawn from N to P . A line OP is drawn from the center to P . The angle between ON and NP is labeled τ . A handwritten note says "Flat phosphor screen".

You see that while we are finding out this, you know information regarding the zone axis and the ND and the you know RD of the sample and we know that Kikuchi pattern is basically on a flat phosphor screen right and this basically should have been on a you know it is a gnomonic projection should have been on a sphere right. It should have been something like this on a sphere right.

So, the difference between the flat phosphor screen and the sphere is basically given by you see the distance NP is equal to ON times of \tan of τ , but to tell you that as because the

lambda of the electron beam is source less, then which is almost equal to ON tau because you see that in case of this kind of diffraction, the distance NP is very close to N and therefore, the NP is equal to almost equal to the arc of that sphere.

So, NP is basically equal to ON times tau. So, while, we are doing this kind of calculations, we are taking an assumption that the diffraction pattern is though gnomonic projection, the distance near the center pattern can be considered to be scattered linearly with the projection angle tau and that is we are considering while calculating the zone axis and the ND and the RD of the of a particular Kikuchi pattern 1 by 1.

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Determining Zone axes

Band 1 $\rightarrow h_1 k_1 l_1$, Axis 12 = $u_{12} v_{12} w_{12}$
 Band 2 $\rightarrow h_2 k_2 l_2$ Axis 23 = $u_{23} v_{23} w_{23}$
 Band 3 $\rightarrow h_3 k_3 l_3$ Axis 31 = $u_{31} v_{31} w_{31}$

Axis 12 = $[u_{12} v_{12} w_{12}] = (h_1 k_1 l_1) \times (h_2 k_2 l_2)$
 $= (\bar{3}1) \times (2\bar{2}0) = (1 \times 0 - 1 \times \bar{2}), -(3 \times 0 - 1 \times 2), (3 \times \bar{2} - 1 \times 0)$
 $= 2, 2, 4 = [112]$

Axis 23 = $[u_{23} v_{23} w_{23}] = (h_2 k_2 l_2) \times (h_3 k_3 l_3)$
 $= 2\bar{2}0 \times 0\bar{2}\bar{2} = (2 \times 2 - 0 \times 2), -(2 \times \bar{2} - 0), (2 \times 2 - \bar{2} \times 0) = [444]$
 $= [111]$

Axis 31 = $[u_{31} v_{31} w_{31}] = (h_3 k_3 l_3) \times (h_1 k_1 l_1)$
 $= (0\bar{2}\bar{2}) \times (\bar{3}1) = (0 \times 1 - \bar{2} \times 1), -(0 \times 1 - \bar{2} \times \bar{3}), (0 \times 1 - 2 \times \bar{3}) = [4, 6, 6]$
 $= [233]$

So, let us consider you know determination of the zone axes right. Now, let us consider that we are trying to determine the zone axis a 12 and then zone axis 23 and zone axis 31. If the band 1 is basically h 1 k 1 l 1; band 2 is h 2 k 2 l 2 and band 3 is h 3 k 3 l 3, where the axis 12 is basically u 12 v 12 w 12; axis 23 is equal to u 23 v 23 w 23 and axis 31 is equal to u 31 v 31 w 31.

Here, it is w and w 31. Then, axis 12 which is equal to you know u 12 v 12 w 12 equal to you know using the right hand thumb rule is h 1 k 1 l 1 cross product with band 2 h 2 k 2 l 2 right. Axis 23 equal to u 23 v 23 w 23, also by using the right hand thumb rule, it becomes equal to h 2 k 2 l 2 from band 2, band 2 cross product with band 3 which is h 3 k 3 l 3 right.

Then, axis 31 equal to $u_{31} v_{31} w_{31}$, again right hand thumb rule and that is band 3 h 3 k 3 l 3 has to be cross product with h 1 k 1 l 1 that is band 1 right. Now, we know that h 1 k 1 l 1 is basically you know $3 \bar{1} 1$ right and cross product with h 2 k 2 l 2 which is $2 \bar{2} 0$ right. And if we do this, you will find that $u_{12} v_{12} w_{12}$ equal to let me do it for you for the first quadrant 1 into 0 sorry minus 1 into 2 bar right comma minus you know $3 \bar{1}$ into 0 into 0 minus 1 one into 2 into 2 and then again, $3 \bar{1}$ this 1 into 2 bar into 2 bar minus you see 1 this one into 2.

So, this makes it equal to you see $2 \bar{2}$ bar, sorry again 2 and then, 6 bar right. So, sorry 3 into 2 is 6; minus of 2 is 4. So, this makes equal to $2 \bar{2}$ and 4 right. Just try to delete this small part to make it proper ok.

So, what I was saying that this is basically 2 from here and then, 2 from here you see minus of 2 minus and then, it is 3 2 just 6, minus of 2 is 4. So, the Miller indices has to be normalized to the smallest Miller indices possible. So, it becomes 1 1 2 right. On the other hand, if you take and find out axis 23, so h 2 k 2 l 2 is band 2 which is basically $2 \bar{2} 0$, $2 \bar{2} 0$ and if you do a cross product with h 3 k 1 l 3 k 3 l 3, it is $0 \bar{2} 2$ bar.

And if we use the same procedure, if you make the same procedure and then, we can find out, then that becomes equal to 2; sorry $2 \bar{1}$ into 2 minus 0 into 2 comma minus of you see 2 into 2 bar minus of 0 comma 2 into 2 minus of 2 bar into 0, which becomes equal to basically 4 4 and 4 and then, it has to be normalized to the smallest Miller indices possible. So, axis 23 becomes 111. So, what do you find out that axis 12 is basically 112; axis 23 is basically 111. Now, let us find out axis 31.

Axis 31 is the cross product between band 3 and band 1 that is a cross product between $0 \bar{2} 2$ bar you know cross product with $3 \bar{1} 1$ which is basically equal to you see 2 into 1 minus 2 bar into 1 right. 2 into 1 minus 2 bar into 1 and then, minus sorry 0 into 1 minus 2 bar into 3 bar comma 0 into 1 minus 2 into 3 bar this becomes equal to you see 4, 6 and again 6 and normalized to the lowest Miller indices, it becomes equal to 233.

So, axis 311 is basically 233 right. So, in this way, we can find out we can determine the zone axis of a from a you know Kikuchi pattern and you see that in order to find out ND and the zone axis and the ND and the RD from a Kikuchi pattern, we basically need only you see 3 bands. So, band 1, band 2, and 3 and we can obtain this, this and this.

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Determining ND/BN

If the angles between the incident electron beam BN and the zone axis is known and are $\alpha_{12} = 11.6^\circ$, $\alpha_{23} = 8.5^\circ$, $\alpha_{31} = 7.2^\circ$

$BN = qrs$

$\cos \alpha_{12} = \frac{(u_{12} v_{12} w_{12}) \cdot (qrs)}{\sqrt{u_{12}^2 + v_{12}^2 + w_{12}^2}} \Rightarrow \cos 11.6^\circ = \frac{112}{\sqrt{1^2 + 1^2 + 2^2}} \cdot qrs$
 $\Rightarrow q + r + 2s = \frac{\sqrt{6}}{\sqrt{6}} \cdot \cos 11.6^\circ = 2.399$ (i)

$\cos \alpha_{23} = \frac{(u_{23} v_{23} w_{23}) \cdot (qrs)}{\sqrt{u_{23}^2 + v_{23}^2 + w_{23}^2}} \Rightarrow \cos 8.5^\circ = \frac{111}{\sqrt{3}} \cdot qrs$
 $\Rightarrow q + r + s = \sqrt{3} \cdot \cos 8.5^\circ = 1.713$ (ii)

$\cos \alpha_{31} = \frac{(u_{31} v_{31} w_{31}) \cdot (qrs)}{\sqrt{u_{31}^2 + v_{31}^2 + w_{31}^2}} \Rightarrow \cos 7.2^\circ = \frac{233}{\sqrt{22}} \cdot qrs$
 $2q + 3r + 3s = \sqrt{22} \cdot \cos 7.2^\circ = 4.659$ (iii)

Now, axis 12 has an angular relationship with ND that is alpha 12 which is 11.6 degrees; axis 23 which is 111 has an angular relationship alpha 23 with respect to ND which is 8.5 degrees; axis 31 which is you know 233 has an angular relationship of alpha 31 which is 7.2 with respect to ND.

Now, the you see the dot product between the two axes is basically equal to the cos of this angles alpha 12 alpha 23 and alpha 31 right. So, just I will write it for you that if the angles between the incident electron beam BN and the zone axis is known and are alpha 1, alpha 2 and alpha 3. Then, if say BN is equal to in Miller indices say it is q r s, then the you know then cos of alpha 12 is equal to the axis 12 which is u 12 v 12 w 12 dot product with q r s.

Now, this is basically divided by u 12 whole square plus v 12 whole square w 12 whole square to normalize the total equal to 1 right. Now, cos of alpha 23, now is equal to then u 23 v 23 w 23 divided by root over u 23 whole square v 23 whole square w 23 whole square times q r s; means dot product of q r s. Cos of alpha 31 is equal to u 31 v 31 w 31 by root over u 31 whole square v 31 whole square w 31 whole square dot of q r and s.

So, now let us calculate one by one this cos alpha q r s for cos alpha 12. So, cos alpha 12 that is you see is cos of 11.6 degrees and if we calculate, I have priory calculated it and this comes out ok, let me calculate it. So, if cos of 11.6 degrees is equal to then you see u 1 v 12 w 12 which is 112 and then, it is root over 1 square plus 1 square plus 2 square.

So, 1 plus 1 plus 4 which is equal to 6. So, I am doing a little step jump to save the space here and so, and it is multiplied. So, it is a dot product with q r s. So, you see we can write this as q plus r plus 2 s is equal to root 6 times cos of 11. 6 degrees and which I have priory calculated and it is equal to 2.399. So, you can use the calculator and see whether it is correct or not.

Now, in this case alpha 23, which is equal to cos of 8.5 degrees equal to; so, alpha 23 the axis u 23 v 23 w 23 is 1 1 1. So, it is 111 divided by how much it is? u square 1 square plus 1 square plus 1 square that is divided by root of 3 times dot product q r s. So, if you see here, this is q plus r plus s equal to root 3 times cos of 8.5 degrees which I have calculated to be equal to 1.713 right.

Now, for cos alpha 31 alpha 31 is basically 233. So, you see cos of alpha 31 which is 7.2 degrees equal to 233 divided by root of 2 square plus 3 square plus 3 square that is 4 plus 9 plus 9 and that is basically equal to root of 22 times q r s becomes equal to. So, 2 q plus 3 r plus 3 s is equal to root of 22 times cos of 7.2 degrees, which I have already done a priory calculation and which is coming out to be equal to 4.659.

So, you see that basically. we have obtained three equations; this is equation number 1, this is equation number 2 and this is equation number you see 3 and from these three equations, we can we have to find out three variables which are q, r and s and now, it is much easier to find from these three equations right.

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Determining ND/BN

$$q + r + 2s = 2.399 \quad \text{--- (i)}$$

$$q + r + s = 1.713 \quad \text{--- (ii)}$$

$$2q + 3r + 3s = 4.659 \quad \text{--- (iii)}$$

→ Subtraction - eq (i) - (ii) ⇒ $s = 2.399 - 1.713 = 0.686$

→ " " " eq - 3(ii) - (iii) ⇒ $q = 3 \times 1.713 - 4.659 = 0.48$

→ " " " eq - (iii) - (ii) - (i) ⇒ $r = 4.659 - 1.713 - 2.399 = 0.546$

$qrs = (0.48, 0.546, 0.686)$

$(0.5, 0.6, 0.7) = [567] \Rightarrow \underline{\underline{ND}}$

$\alpha_{12} = 11.6^\circ$
 $\alpha_{23} = 8.5^\circ$
 $\alpha_{31} = 7.2^\circ$

So, in this way, we have obtained three equations with three variables from which we need to find out these three variables; these are q , r and s which are Miller indices for the ND right. So, if you write the first equation, what we obtained is q plus r plus $2s$ equal to 0.2399 . This is equation number 1 obtained with zone axis 12. The second equation is q plus r plus s equal to 1.713 obtained with the zone axis 23 and the third equation is $2q$ plus $3s$ plus $3r$ plus $3s$ equal to 4.659 which is obtained between ND and the zone axis 31 which is which is 233 right.

So, now, if we do the subtraction between you know equation 1 with equation 2, you see equation 1 is q plus r plus $2s$ and equation 2 is q plus r plus s . So, if you subtract q plus r plus $2s$ minus q minus r minus s , then it remains only s which is equal to 2.399 from equation 1 minus of 1.713 , which comes out to be equal to 0.686 .

Now, if you do a second subtraction, let us do a second subtraction between equation you see if we take the equation number 2 and multiply first with 3 right and then, if we subtract the equation number 2 with the equation number 3. Then, what will happen? You can see that $3q$ plus $3r$ plus $3s$ is subtracted that is minus of $2q$ minus $3r$ minus $3s$ which gives you the value of q which is equal to you know 3 times 1.713 minus of 4.659 right. So, this becomes equal to you see 0.48 .

Now, we do another subtraction; but now, you see if we do the subtraction for equation you know we take equation 3 and subtract this with equation 2 and then, we subtract this with equation 1, then what will happen? You see $2q$ plus $3r$ plus $3s$ of equation 3 is subtracted from $2q$'s of equation 1 and 2, $2q$ $2r$'s of equation 1 and 2 and $3s$ from equation 1 and 2.

Therefore, we get the value of r which remains here and this becomes equal to 4.659 minus equation number 2 that is 1.713 minus 2.399 and this basically is equal to 0.546 . So, the value of q r s which is the Miller indices of ND that is the incident electron beam BN, it becomes equal to you see 0.48 , 0.547 that is r and s is 0.686 .

Now, you see if we make it closer to the you know if you remove try to remove its decimal and try to make it closer, then you see you can write it its 0.5 and 0.6 and 0.7 . So, the Miller indices of the q r s is basically close to 5, 6 and 7 and that is how we can find out the you see the ND of the sample. Now, you remember that while we have found the ND which is equivalent to the beam normal of the sample; the sample is kept in such a way that the RD and the TD is basically known.

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Determining RD

of the TEM sample is kept with reference direction RD (or TD) // to the edge of the specimen holder.

↳ Copper grid.

→ holder can be used for image rotation → along a certain sample reference direction.

RD → we will get a new kikuchi pattern with a different ND → (q, r, s)

$$[q, r, s] \times [q_1, r_1, s_1] = [l, m, n]$$

Miller indices for RD.

Tilting the sample about RD, we find out a new ND → product of old ND with new ND → will give RD.

And let us see how we can obtain the value of RD in this sample right. So, in order to find out RD of the sample, in order to find out determine this RD when the you know q, r, s of a certain Kikuchi pattern is known. So, you see that in case of TEM, if the sample is kept in such a way that the RD and the TD is known as I was saying in the last slide. So, let us let me write it down that if the TEM sample basically is kept in such a way that with I mean it is in reference, it is in reference direction RD or TD parallel to the you know the edge of the you know specimen holder.

We know that in case of TEM, the specimen holder you know the specimen holder is something like a you know copper grid right; copper grid right. It looks something like this, let me try to draw it something like this. It has something grids on it. So, something like a copper grid and this holder can be you know utilized can be used for meaning you know image rotation.

So, you know one can rotate the image, if we know say for example, if say we have kept the sample in such a way this is RD and say for example, this is TD, one can rotate the image, rotate the you know copper grid along RD about RD right something like that.

Now, if you say that if this is RD and then, this is TD of the sample inside the screen and this is ND and if we get the opportunity to you know rotate you see RD say we are rotating RD like this. And then, the ND after the rotation basically changes right. So, the Kikuchi pattern basically changes right. So, if we can holder can be used for rotation along a certain you

know sample reference direction, we will get you know a new Kikuchi pattern right; a new Kikuchi pattern which will have a with a which will have a different ND; that means, a different q r s . Let us say it is q 1 r 1 s 1 this time right.

So, if we can rotate the specimen along a certain RD, then we can get a new Kikuchi pattern and this Kikuchi pattern will have a you see a different ND right; q 1 r 1 s 1 and then, we can for the new Kikuchi pattern, we can find out this q 1 r 1 s 1 like how we have determined in the last few slides. So, once we can determine this q 1 r 1 s 1 , we can do a cross multiplication of the previous q r s with the you know cross product with the q 1 r 1 s 1 will give the you know the Miller indices say it is you know l m n that is the you know Miller indices for RD.

Because while we rotate the specimen, the ND is changing and the TD is changing; as the rotation is carried out along RD, the RD is not changing. So, one ND which is q r s and another ND which is you know q 1 r 1 s 1 and the cross product between one with the another will give you this direction which is RD in terms of its Miller indices. So, tilting the sample along about RD, we can find out a new ND which is this and then, cross product of old ND with new ND that is cross product sorry product of h of the Miller indices of new and the old ND will give RD.

But you see that while determining RD, we cannot do it for if means it is not practical to determine RD like this right for every electron incident beam position and then, go to the next point for higher studying and do the same tilting, its a very tedious process to do it. So, one has to find out RD without rotating the sample and using a single Kikuchi pattern right.

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Determining RD from a Kikuchi pattern

→ Young et al [1973] and Heilmann et al. [1982]

$x = hkl$
 $y = uvw$
 $z = ND = qrs$

Rotation matrix, R_{CP}
 from crystal frame of reference
 to the pattern frame of reference [intermediate]

is $R_{CP} = \begin{bmatrix} x & y & z \end{bmatrix} = \begin{bmatrix} h & u & q \\ k & v & r \\ l & w & s \end{bmatrix}$

The pattern frame of reference P^* contains the information of the indexed beam normal (BN/ND) and differs from the sample reference system by some rotation angle, γ along ND/BN.

So, let us try to understand how we can determine RD from a single Kikuchi pattern and let us take the same example and let me let me draw the Kikuchi pattern this time for you and say this is the Kikuchi pattern and as I said that this is the RD and this is the TD and somewhere, there is you know of course, ND is something like this.

Now, if you see that if the Kikuchi pattern is say for example something like this. Say it is one of the Kikuchi pattern that is from that figure that I was showing. Now, if we know that perpendicular to the Kikuchi pattern, if there is a you know vector or a direction perpendicular to the Kikuchi pattern.

Let us say this is x and if we can find out the you know hkl of this the Miller indices of this direction, you see sorry this direction. Let us say that in this example, if we have a direction x like this and then, the direction which is parallel to this Kikuchi band, let us say it is y and let us say that it is uvw and w right. This direction is uvw . z of this x y and z axes is equal to ND and let us say that ND as usual is qrs right and this is z which is parallel to ND right. Now, you see this is this can be considered as a pattern reference system right.

So, this can be considered as pattern reference system and this pattern reference system can be you know calculated means a rotation matrix can be calculated between the you see the pattern reference system and the you know crystal reference system because the Miller indices of this x , y and z are known and so, this method that we are trying to tell is because of

the development by research and development by various groups; one is Young et al, who started their work in 1973 and published them in 1973 and another is Heilmann et al 1982.

So, you see that both of them in their group, they separately try to find out RD from a Kikuchi pattern and they come up with a solution which is similar like this and you see that as x equal to you see $h k l$ and you see y equal to $u v w$ and z equal to ND of course, that is $q r s$; then, the rotation matrix you see, then the rotation matrix that is you know R_{CP} , the rotation matrix from you know crystal frame of reference to the you know pattern frame of reference you know Kikuchi pattern frame of reference and this pattern frame of reference is basically an intermediate frame of reference right.

So, the rotation matrix from the crystal frame of reference to the pattern frame of reference is given by this R_{CP} and can be given by matrix something like this, which is basically x let me write $x y$ and z and which is equal to x is $h k l$, y is $u v w$ and z is $q r$ and s .

So, the pattern frame of reference P , let me write it down. The pattern frame of reference that is ' P ' contains the information of the indexed beam normal that is BN or ND and differs from the sample reference system by some rotation angle. And say that that rotation angle say this is the direction of RD and say this rotation angle is γ right and this rotation angle is along the beam normal right; ND.

So, you see that we can have a rotation matrix from the crystal frame of reference to the pattern frame of reference like this right.

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Determining RD from a Kikuchi pattern

If this pattern reference system is denoted by $1'2'3'$
 x is $1'$, y is $2'$, z is $3'$

If the sample reference system is denoted by $1, 2, 3$
for RD, TD & ND, respectively

Then the rotation matrix from the pattern reference system to the sample reference system

$$R_{ps} = \begin{bmatrix} x.RD & x.TD & x.ND \\ y.RD & y.TD & y.ND \\ z.RD & z.TD & z.ND \end{bmatrix} = \begin{bmatrix} 1',1 & 1',2 & 1',3 \\ 2',1 & 2',2 & 2',3 \\ 3',1 & 3',2 & 3',3 \end{bmatrix} = \begin{bmatrix} \cos\gamma & \cos 90^\circ - \gamma & \cos 90^\circ \\ \cos(90^\circ + \gamma) & \cos\gamma & \cos 90^\circ \\ \cos 90^\circ & \cos 90^\circ & \cos 0^\circ \end{bmatrix}$$

$$= \begin{bmatrix} \cos\gamma & \sin\gamma & 0 \\ -\sin\gamma & \cos\gamma & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

Now, if we try to determine the rotation matrix between the pattern frame of reference and sample frame of reference, it will be quite easy. But let me again take the time to you know draw the same thing here and let me say ok, this is the Kikuchi band and this is the center line and this is the x axis that we were drawing right and say this is the y then and so, let us say that this is RD and this is TD right.

And let us say this is as ND which is equal to z and same for the for both the cases right. So, if we look into this, if this pattern reference system is denoted by you know say 1 dash, 2 dash, 3 dash that is x x is 1 dash and y is 2 dash and z is 3 dash.

On the other hand, if the sample reference system is denoted by 1, 2, 3 for you know RD, TD and ND respectively. Then, the then you see then the rotation matrix, then the rotation matrix from the pattern reference system to the sample reference system is you know can be given by R you know PS and which is equal to you see and let me give a brief work here.

So, as z and ND is same. So, z dot product with ND will be here; of course, it will be here and if as because the rotation is basically along the z and by an angle which is gamma, then that is the dot product between see, initially, it will be the relationship between the pattern and the sample.

So, the dot product is between x that is the x for the pattern dot product with RD, the second will be x for the pattern with respect to the TD and then, x for the pattern with respect to ND

right; third will be y with respect to RD, then y with respect to TD, then y with respect to ND and then, z with respect to RD z with respect to TD and like I said z with respect to ND.

This from the if we take the above 1 bar toward 3 bar and 1, 2, 3 reference system, we can write it something like that $\bar{1}_1, \bar{1}_2, \bar{1}_3, \bar{2}_1, \bar{2}_2, \bar{2}_3, \bar{3}_1, \bar{3}_2, \bar{3}_3$ that is all of them are basically dot products right and therefore, we can write.

So, dot products between you know x and RD is basically equal to you see \cos of γ obviously, and dot product between x and TD will be equal to you see \cos of 90 minus γ , sorry 90 minus γ and dot product between you see x and ND is \cos of 90 which is basically 0 degrees right; dot product between you see y , this is y and RD is equal to \cos of 90 plus γ ; dot product between y .

And TD is basically again \cos of γ . Because you see if this is γ then the angular relationship between y and TD is again γ . The relationship between y and ND is \cos of 90 degrees; the relationship between z and RD is \cos of 90 degrees; the relationship between z and TD is again 90 degrees. So, \cos of 90 degrees and relationship between z and ND that is \cos of 0 degree is this one.

So, the rotation matrix pertaining to you know the pattern reference system with respect to the sample reference systems comes out to be equal to \cos of γ \sin of γ 0 minus of \sin of γ \cos of γ 0 0 0 1 and obviously, this will be like this because you see the rotation is along ND which is equal to z , therefore, it will be 1 and this is the rotation matrix.

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Determining RD from a Kikuchi pattern

Now, rotation matrix from the crystal reference frame to the sample reference frame

$$R_{CS} = R_{CP} \cdot P_{BS}$$

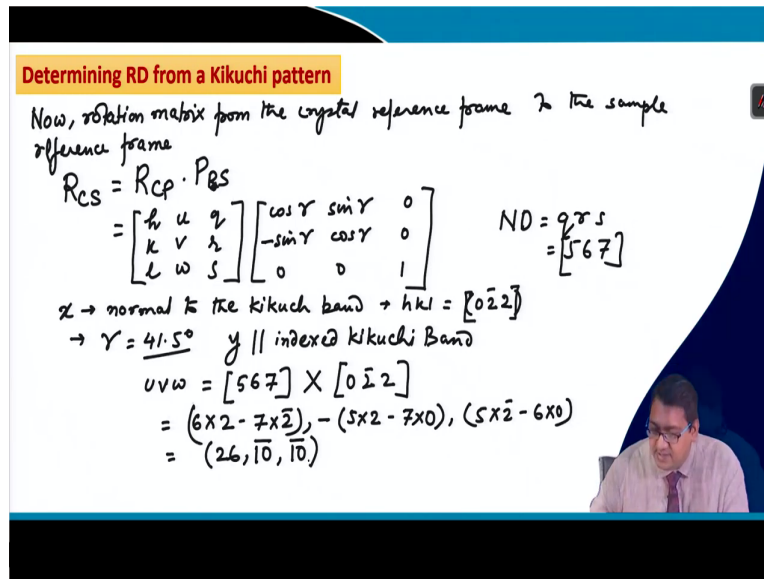
$$= \begin{bmatrix} h & u & q \\ k & v & r \\ l & w & s \end{bmatrix} \begin{bmatrix} \cos \gamma & \sin \gamma & 0 \\ -\sin \gamma & \cos \gamma & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad ND = qrs = \begin{bmatrix} 5 & 6 & 7 \end{bmatrix}$$

$x \rightarrow$ normal to the Kikuchi band $\rightarrow hkl = [0\bar{2}2]$

$\rightarrow \gamma = 41.5^\circ$ $y \parallel$ indexed Kikuchi Band

$$uvw = [567] \times [0\bar{2}2]$$

$$= (6 \times 2 - 7 \times \bar{2}), -(5 \times 2 - 7 \times 0), (5 \times \bar{2} - 6 \times 0)$$

$$= (26, \bar{10}, \bar{10})$$


Now, if we look further into this and sorry and if we try to determine further, now the new rotation matrix that we need to obtain is between the you know crystal reference frame and the sample reference frame right. So, now, if we say rotation matrix from the you know crystal reference frame to the you know important sample reference frame. Sorry for the handwriting that will be R CP right sorry R CS right and this should be equal to R CP times R PS; R PS right.

Now, R CP as we calculated is h k l, u v w, q r s right and R PS that is pattern to sample is cos of gamma, sin of gamma right, minus of sin of gamma, cos of gamma, 0 0 1, 0 0 like this right. Now, if we say that we know that what is h k l because h k l is perpendicular to a Kikuchi pattern which is you know 0 2 2 bar. So, the h k l that is x which is normal to that the Kikuchi band.

So, we know that this h k l is equal to you see 0 2 bar 2 from the Kikuchi pattern. Now, if say for this example the angle gamma is equal to 41.5 degrees ok and I am not changing anything here and I am referring it to the book and the I am I am using the same angle so that one can go and read the book and it becomes easier for them right.

So, if y is basically parallel to that Kikuchi band you know that indexed Kikuchi band and do you already know the value of you see ND right. So, we know the value of ND is equal to you see q r s equal to 5 6 and 7 right and we calculated that. Let me change it into direction symbol. So, what could be the Miller indices of y? So, by doing a cross product of you know

using a right hand thumb rule between the x and ND, one can obtain the value of you know in the Miller indices of y.

So, u v w which is the Miller indices of y is equal to the cross product between ND that is 5 6 7 cross product into what is this h k l 0 2 bar 2. Now, if we calculate this it comes out to be 6 into 2 minus 7 into 2 bar for the first one; then minus of you see 5 into 2 minus 7 into 0 comma 5 into 2 bar minus 6 into 0 right.

So, this comes out to be equal to be 26, 10 bar, 10 bar right. So, you see that we have calculated the value of h k l from the value of Miller indices of y which is u v w and the Miller indices of ND which we have calculated earlier.

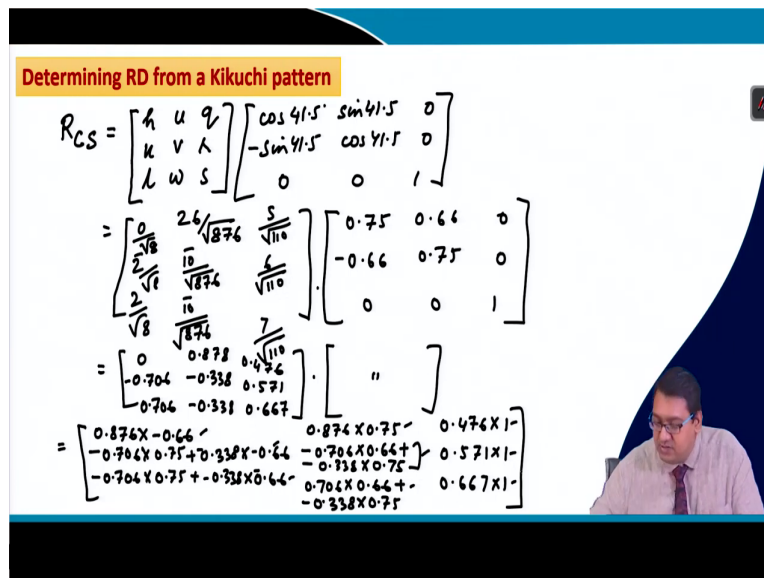
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Determining RD from a Kikuchi pattern

$$R_{CS} = \begin{bmatrix} h & u & q \\ k & v & r \\ l & w & s \end{bmatrix} \begin{bmatrix} \cos 41.5^\circ & \sin 41.5^\circ & 0 \\ -\sin 41.5^\circ & \cos 41.5^\circ & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

$$= \begin{bmatrix} \frac{0}{\sqrt{8}} & \frac{26}{\sqrt{876}} & \frac{5}{\sqrt{110}} \\ \frac{2}{\sqrt{6}} & \frac{10}{\sqrt{876}} & \frac{6}{\sqrt{110}} \\ \frac{2}{\sqrt{8}} & \frac{10}{\sqrt{876}} & \frac{7}{\sqrt{110}} \end{bmatrix} \begin{bmatrix} 0.75 & 0.66 & 0 \\ -0.66 & 0.75 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

$$= \begin{bmatrix} 0 & 0.878 & 0.411 \\ -0.706 & -0.338 & 0.571 \\ 0.706 & -0.338 & 0.667 \end{bmatrix} \begin{bmatrix} " \\ " \\ " \end{bmatrix}$$

$$= \begin{bmatrix} 0.876 \times 0.66 & 0.876 \times 0.75 & 0.476 \times 1 \\ -0.706 \times 0.75 + 0.338 \times 0.66 & -0.706 \times 0.66 + 0.338 \times 0.75 & 0.571 \times 1 \\ -0.706 \times 0.75 + 0.338 \times 0.66 & -0.706 \times 0.66 + 0.338 \times 0.75 & 0.667 \times 1 \end{bmatrix}$$


So, once we found out the value of you know the value of Miller indices of y and the value of Miller indices from the value of Miller indices of x and z which were already there, then we can get the rotation matrix between the crystal and the sample coordinate system which I have written in the previous slide as h k l, u v w, q r s times you know cos of you see 41.5 degrees sin of 41.5 degrees 0 minus of sin of 41.5 degrees cos of 41.5 degrees 0 and then, 0 0 1.

Now, if we write the values of h k l, u v w, normalize it to its you know h square plus k square plus l square in case of h k l; u square plus v square plus w square in case of u v w and q square plus r square plus square in case of q r s, then you see what we will get. We will get

in case of $h k l$, it is 0 you know $2\bar{2}$ and 2 and it will be divided by you see root of 8 right because $2^2 + 2^2$ is equal to 4 plus 4 and root over 8.

So, root over 8 and here also root over 8. In case of $u v$ and w , it is $26, 10\bar{10}$ and $10\bar{10}$ and if we calculate, the it will be square root of $26^2 + 10^2 + 10^2$ and if you calculate you will find out that it is coming out to be root over 876. So, we will divided by root of 876 in each case right and then, $q r s$ is equal to $5\bar{6}$ and 7 and so, root over $5^2 + 6^2 + 7^2$ and it comes out to be 110. So, we will divided it by 110 right.

And then, it is dot product with respect to you see \cos of 41.5 is 0.75, \sin of 41.5 is 0.66, next is $0\bar{0.66}, 0.75, 0\bar{0}0\bar{1}$. Now, if we do a dot product of it, what we will find out that this becomes equal to you see $0, 0.706$ it is, it will be minus because it has a root 2 and then, 0.706 here and then, it is 26 divided by root of 876.

It comes out to be 0.878 and then, 10 divided by root of 876 comes out to be minus of 0.338, minus of 0.338 here also. And then, 5 divided by root of 110 comes out to be 0.476, it also comes here 0.6 divided by root of 110 comes out to be root of 571 and then, root of 0.667 right and dot product with you see this one.

So, if we do it and we can find out this equal to you see it is a big one. So, 0.876 into minus of 0.66 plus of minus of 0.706 into 0.75 you know plus 0.338. So, minus of this into minus of 0.66 and for the third case, it will be minus of 0.706 again into 0.75 plus of minus 0.338 into 0.66, it is also minus right. And for the second quadrant, it will be 0.876 into 0.75 and then, it will be for the second one minus of 0.706 into 0.66 plus minus 0.338 into 0.75.

So, this is one and then, the third one is 0.706 into 0.66 plus minus 0.338 into 0.75. For the third quadrant, it will be it will be little easier. Because 0.476 into 1, 0.571 into 1 and then, 0.667 into 1. So, you see that we can get the rotation matrix between the you see the crystal coordinate system and the sample coordinate system. So, by in this way, we have obtained the 3 cross 3 matrix containing 9 variables. So, you see 1, 2, 3, 4, 5, 6, 7, 8, 9.

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Determining RD from a Kikuchi pattern

$$Res = \begin{bmatrix} \overset{RD}{-0.579} & \overset{TD}{0.659} & \overset{ND}{0.476} \\ -0.307 & -0.719 & 0.571 \\ +0.753 & 0.212 & 0.667 \end{bmatrix} \begin{matrix} 5 \\ 6 \\ 7 \end{matrix}$$

$$ND \text{ qrs} = [567]$$

$$RD = \left[\frac{-0.579}{0.307}, \frac{-0.307}{0.307}, \frac{0.753}{0.307} \right]$$

$$= [-1.89, -1, +2.45]$$

$$= [-20, -10, 25]$$

$$= \underline{[-4 -2 5]} \checkmark$$

And if we calculate this and solve it, we will find out that these variables are basically coming out to be 0.579, 0.659 and 0.476 and then, 0.307, 0.719 minus 0.571 and then plus 0.753, 0.212 and 0.667. So, basically, this is the rotation matrix between the crystal coordinate system and the sample coordinate system.

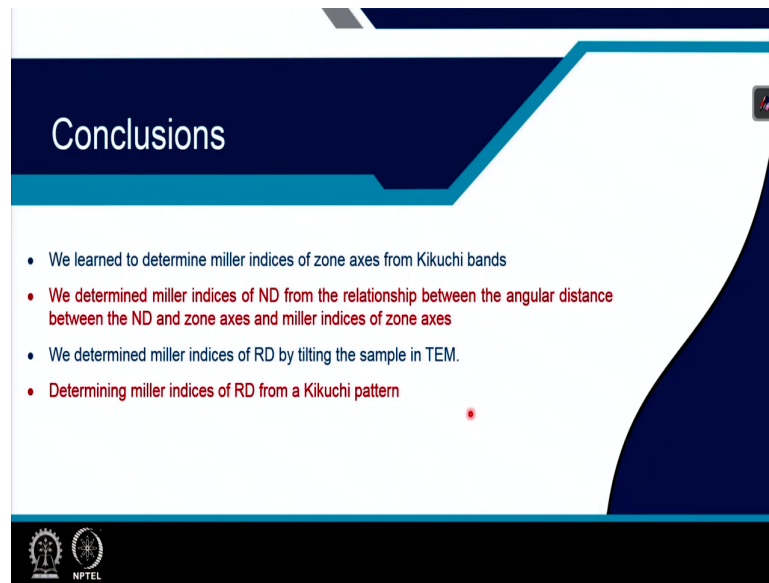
And therefore, we can say that these are the you know RD, TD and ND of the sample and you can see that this is 5 6 and 7 for the q r s of ND right. So, in this way, we have obtained, you can find we have found out the value of RD in terms of you know h k l which is basically equal to minus of 0.579 minus of 0.307 and then 0.753.

Now, let us find out this Miller indices in terms of closest you know integers and for that, it is very easy to do it you let us divide this whole thing by you know you see 0.307 for example. So, you see 0.307 and then, 0.307. So, what happens that it will come out to be minus of 18.9 minus of 1 and minus of you see 8; 1.89 and this is plus of 2.45.

So, if we find out a closer solution, then it becomes equal to 2. Sorry. Let us say we multiply it by 10, then it becomes equal to 18.9 which is basically near to 20 and then, it is minus of 10 because we are multiplying it by 10 and then, it becomes equal to 25. So, if we divide this by 5, then it becomes 4, 2, 5.

So, something like this will be the value of RD and that is why we find out the value of RD, without rotating the Kikuchi pattern from a single Kikuchi pattern right.

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Conclusions

- We learned to determine miller indices of zone axes from Kikuchi bands
- We determined miller indices of ND from the relationship between the angular distance between the ND and zone axes and miller indices of zone axes
- We determined miller indices of RD by tilting the sample in TEM.
- Determining miller indices of RD from a Kikuchi pattern

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So, in this lecture, we learned to determine the Miller indices of the zone axis of the Kikuchi bands, we determined that Miller indices for the ND from the you know angular relationship between the zone axis and the ND which is basically dot product.

We determined the Miller indices of RD by you know tilting the sample in the using the sample holder in the TEM and finally, we use the Young's and the Heilmann's approach to determine the you know value of RD, TD and ND, without rotating the Kikuchi or by using a single Kikuchi pattern. Thank you very much for this class.