Texture in Materials
Prof. Somjeet Biswas
Department of Metallurgical and Materials Engineering
Indian Institute of Technology, Kharagpur

Module - 03
Texture representation
Lecture - 12
Three Dimensional Texture Analysis

Good day, everyone. Today is the 12th lecture of the course Texture in Materials and we will do Three Dimensional Texture Analysis.

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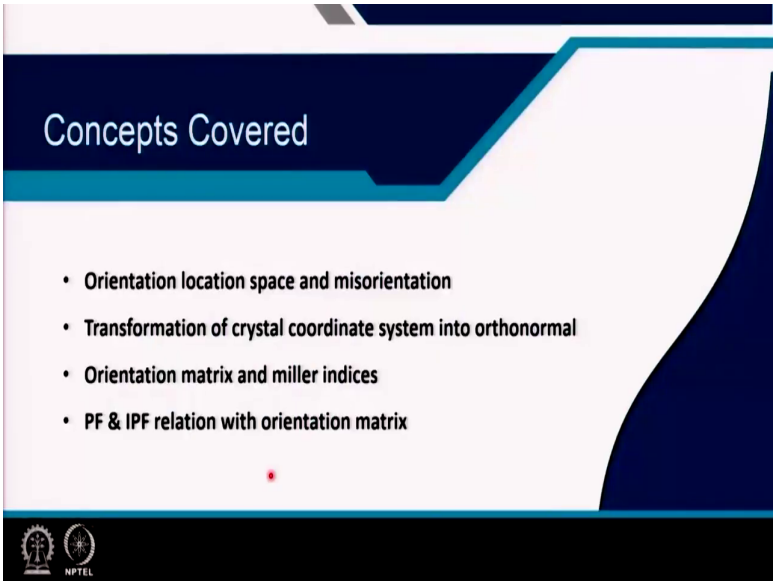

The concepts that will be covered in this course lecture will be: orientation location space and misorientation. Second, transformation of crystal coordinate system into orthonormal, which is required to relate it with the sample coordinate system in order to obtain the texture. Third, orientation matrices and miller indices, pole figure and inverse pole figures relationship with the orientation matrix.

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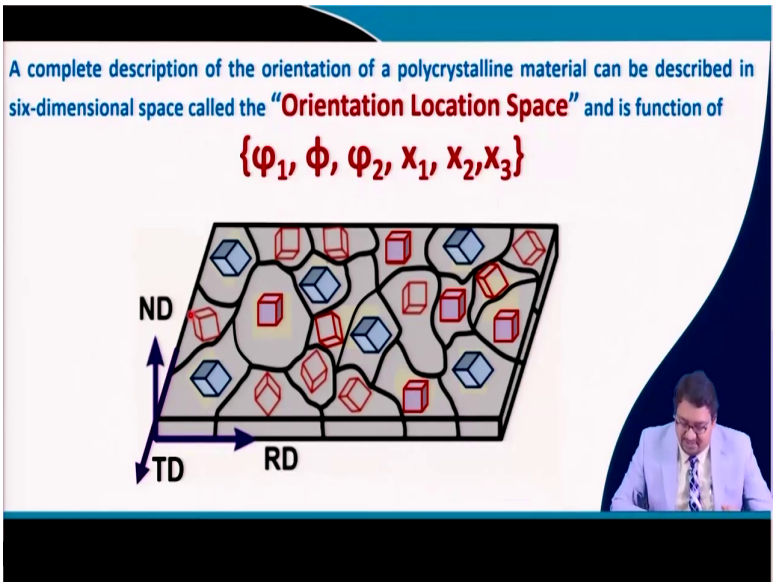

In order to obtain a complete description of the orientation in a polycrystalline material it has to be described in terms of six dimensional space and this is known as the "Orientation Location Space." And the orientation location space consists of a function of six variables and these six variables are phi 1, phi, phi 2, x 1, x 2 and x 3. Therefore, phi 1, phi, phi 2 are the angular variables and x 1, x 2 and x 3 are the locations. So that if we have a polycrystalline material as shown in the example below the schematic below; it has a number of grains and each grain has a different orientation and in these grains there may be some orientation whose which might be present in a larger intensity or larger fraction.

These grains, which have the similar kind of orientation are spatially separated out, but will come as an higher intensity while we will do our texture analysis right or texture measurement right. So that, what do you mean by the orientation location space? Say for example, if we take this particular plate or sheet metal with sample reference direction x as RD y as TD and z as ND and say for example, these are the most important sample reference directions. So, if we have the information of each point or each pixel that is possible the smallest pixel possible within this whole micro structure. So, if we have an information from here from here from here. And, if we go like that raster the whole microstructure and get information from the whole microstructure.

Then not only have we got the information of the texture in terms of phi 1, phi, phi 2 in from each of this pixel, but we also get the information of the x and y. On the other hand, if we do

a three dimensional structure analysis by using say for example, electron backscattered diffraction in a scanning electron microscope like this and then we do an iron beam milling. Therefore, that we can dig a little deeper into the surface and do another electron backscatter diffraction and dig and do another electron backscatter diffraction. So, that we obtain the information from the z-axis inside the sample. So, x y and z or x 1, x 2 and x 3 information. Therefore, we have from each pixel phi 1, phi, phi 2, x 1, x 2 and x 3.

Thereby, we get not only the information about the whole texture of the material information of the texture at each and every point possible and the difference in the orientation or the difference in the texture between each pixel point which will lead for us to know the misorientation of the geometrically necessary boundaries, grain boundaries etcetera.

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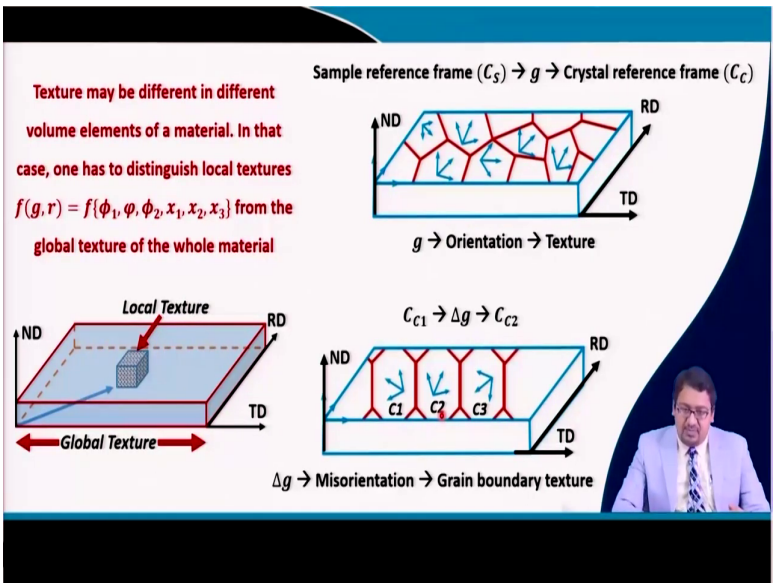

Now in a material which is processed by some way right like solidification deformation the there may be heterogeneity present in the material right. The texture is different in different volume elements of the material right also it will be different in different positions of the material. So, what happens that in that case one has to distinguish this orientation location space that is f in terms of orientation g and in terms of the position of it that is x 1, x 2 and x 3. So orientation location space which is f times function of g and r where g is related to phi 1, phi, phi 2 and r is related to x 1, x 2 and x 3 is related to obtain the local texture because such kind of information can be obtained only from a very small space right. And using an fib one can go below the surface and obtain the information from a small volume of the material,

but the texture obtained from this volume of the material is known as the local texture whereas, the information from the whole material or a large sampled area of the material is known as the global texture. Both local texture and global texture information is important, but local texture includes the information of the orientation location of space in sixth dimension where one can get the information of the orientation also the misorientation.

Whereas, global texture which is obtained usually by X-ray diffraction method by using normal X-rays produced in the laboratories or in from the synchrotron X-rays or from neutron diffraction method of we can obtain the information from deeper in the material from a larger area in the material and this could lead to the overall information of the sample. So, there could be a difference in the texture obtained by the global texture method and the texture obtained by the local texture method. Now, that if we go into more deep into the definition of the texture. Now, if we say that ok that there is a material with a number of grains present in it and each of these grains will have certain orientation and the sample reference direction x 1, x 2 and x 3 or x, y and z are RD, TD and ND.

Then that the relationship between the sample reference system C s; I have said C s and the crystal reference system C c is given by the orientation space which is g and g is known as the orientation space or the orientation matrix and this gives the information of the texture right. On the other hand, if that if we obtain the information in terms of orientation location space then one can obtain the information between the 2 grains right the orientation difference between the 2 grains. If we have the crystal reference system for the grain C1 and the crystal reference system for the grain C2; then we can get delta g, which is the orientation difference between the 2 gains or the mismatch between mismatch of the orientation of the 2 grains.

So, delta g is known as the misorientation right that is the texture of the grain boundary. In this type of case, we can obtain the grain boundary texture between C2 and C3; that is the adjacent grain. Even if there is orientation difference in the in a single grain then there would be a misorientation which will because which may form because of the formation of the low angle boundaries, which is agglomeration of dislocations leading to form geometrically necessary boundaries right.

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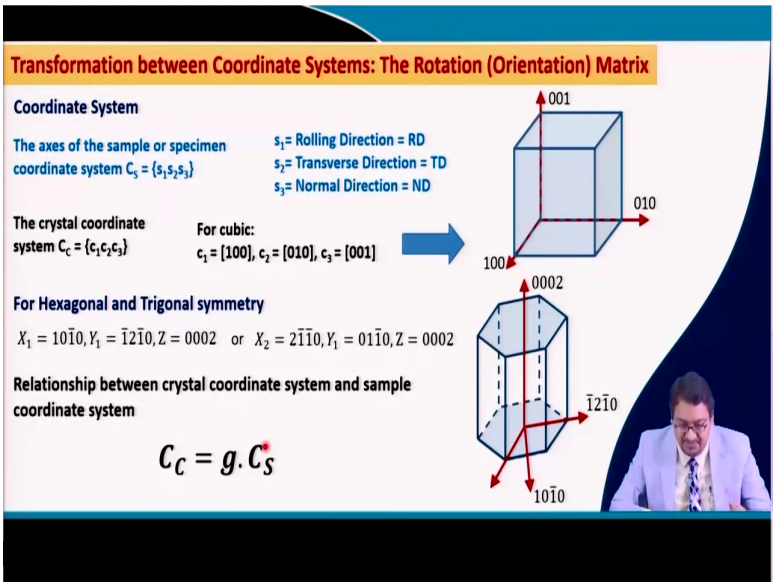

So, when we measure texture and as we said the texture is the relationship between the sample coordinate system and the crystal coordinate system. We see that, the sample coordinate system that is here the axes of the sample coordinate system s 1, s 2 and s 3 right, C s equal to s 1, s 2 and s 3 which in most of the case we used are rolled sample or a material, which has been rolled right.

We use s 1 is equal to rolling direction that is RD, s 2 is equal to transverse direction that is TD and s 3 as a normal direction that is ND and these three important sample axeses are actually orthonormal to each other right. So, they are at 90 degrees to each other. Now, in case of cubic crystals the crystal coordinate system C c; c 1, c 2 and c 3 which is c 1 is equal to 100, c 2 010 and c 3 001 here is the schematic of it and this is also in the orthonormal system. It is very easy for to find out the value of the g which is the orientation matrix relating the sample reference system which is orthonormal to the crystal reference system which is again an orthonormal right. Now, in case of hexagonal and trigonal symmetric crystals what happens is that for example, a nice example of hexagonal system I will give that this is a hexagonal unit cell and that if we keep X as 101 bar 0 then in order to make it orthonormal the Y becomes 1 bar to 1 bar 0 right and Z is 002.

So, here the hexagonal system which follows the miller wave indices has the a axeses that is 112 bar 0 axeses at 120 degrees to each other and we need to convert that into an orthonormal system crystal system. So, that one can relate it to find with the sample

coordinate system to get those value of g. So, that either you have to use X as 101 bar 0 and Y as 112 sorry 1 bar to 1 bar 0 or we have to use a 2 bar sorry 21 bar 1 bar 0 and 011 bar 0 with the Z which is 002 making it 90 90 and 90 degrees.

See therefore, we have for the hexagonal closed packed system to different crystal specimen axis where X and Y can be interchange. And so, while we relate the hexagonal crystal system with the sample we have to initially denote that what is X and what is Y right. Otherwise, the results coming from different sources different researchers or different scientists will not match and will may create a confusion, right.

So, that as because as I said that the relationship of the sample coordinate system and the crystal coordinate system is given by the value g which is the orientation matrix and we usually use that C c is equal to orientation matrix g in terms of C s which is the sample coordinate system.

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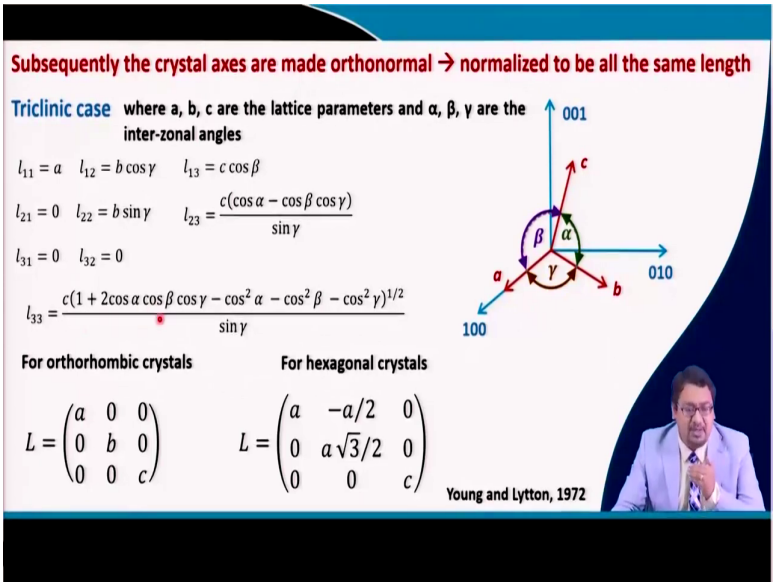

Now, subsequently if any crystal is does not have the orthonormal crystal system that is a its lattice parameter are equal and the angle between the lattice parameter is equal to 90 degree then it has to be made orthonormal and it has to be normalized to the same length.

So, if we take a triclinic system where the you have to see this schematic where a, b and c are not of equal length and then the angles between them alpha, beta and gamma are not equal angles right. Now, this has to be converted into orthonormal system with lattice parameter

equal that is the normalized to the same length and the angles has to be 90 degrees. If we superimpose a lattice parameter is a orthonormal crystal system 100, 010 and 001; then we found find out that we can superimpose it in such a way such that the a coincides with the 100, then there will be a difference in the the axes 010 with b, c and 001 also with the b and c and this is given in the figure which is self explanatory right.

So, if we find out the relationship matrices between relationship matrix between this a, b, c and 100, 010 and 001 which is why it is like this? Because it is normalized to a unit length. So, we obtain the value there will be six values of this matrix and let us say these are l 11, l 12, l 13, l 21, l 22, l 23, l 31, l 32, l 33. So, that l 11 is equal to a because it lies along the same direction as the a. Whereas, l 12 that is the relationship of 100 with respect to this b vector is equal to b times cos of gamma because this is the angle between 100 and b whereas, l 13 is the relationship between 100 and the c which will be b time b times cos of beta.

Now, l 21 is equal to relationship between 010 and a; which is a cos of 90 degree and so, it become 0, l 22 becomes b of the sin of gamma right; l 23 becomes a relationship a little complex relationship c times cos of alpha minus cos of beta cos of gamma divided by sin of gamma right. Whereas, l 31 which is between 001 and alpha is again sorry and a which is again a times cos of 90 degrees is 0, l 32 which is again b times cos of 90 degree is 0 and l 33 is equal to c times 1 plus 2 cos alpha cos beta cos gamma minus cos square alpha minus cos square beta minus cos square gamma to the power half by sin of gamma. This can be calculated and is given in a very old work by Young and Lytton which has been published in 1972. So, that using this matrices containing this nine variables l 11, l 12, l 13, to l 33 we can obtain that for orthorhombic crystals the L is equal to a b and c in the diagonals rest all are 0 because in the orthorhombic crystals a is not equal to b is not equal to c rest alpha beta and gamma is 90 degrees.

In case of hexagonal crystals L becomes equal to l 11 becomes a whereas, l 12 is equal to minus a by 2, l 13 is 0 and l 21 is 0, l 22 is a root 3 by 2, l 23 is 0, l 31 and l 32 will be 0. As we found out and l 33 is equal to c because c is at 90 degrees to both 112 bar 0 and 101 bar 0 of the hexagonal close packed system. Now, this is how we use the Young and Lytton's method to convert the different crystal systems, non-orthonormal crystal systems into orthonormal crystal systems. So, that the relationship C c is equal to g times C s could be obtained between two orthonormal systems right. So, the relationship between the texture could be obtained.

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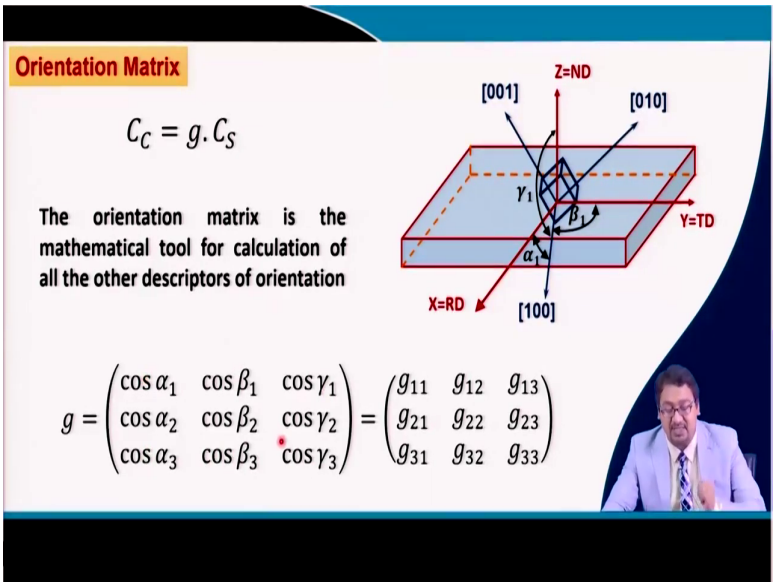

So, that what is an orientation matrix. As I said that, the relationship between the sample coordinate system and the crystal coordinate system angular relationship is the orientation matrix. And it is given by C c is equal to g times C s. So, if we look into a schematic like this the to find out orientation matrix let us say that there is a specimen which has a rolling direction coming out of the the screen and then on the right side it is TD and vertically it is ND.

Therefore, X Y and Z the important sample reference direction RD, TD and ND are at 90 degrees to each other like this. Say for example, this is a polycrystalline material and there are number of grains in it and many grains are having different orientations or different texture, but say of grain is present with this kind of a texture right.

So, the inner cell is oriented in this manner. Therefore, the important crystal reference directions for this kind of orientation or this unit cell can be given by 100 in this direction 010 in this direction 001 in this direction right. So, now that the orientation matrix is the mathematical tool for calculating for calculation of all the description of the orientation that how it is. It is because if g is the orientation matrix then the relationship of 100 with respect to X is cos of alpha 1 because the angle between X and 100 is alpha 1 right. On the other hand, the relationship between Y and 100 that is TD and 100 is beta 1. So, it is cos of beta 1. So, the relationship can be given from in the g 11 which is cos of alpha 1 is the relationship between RD and 100, cos beta 1 is the relationship between TD and 100 cos gamma 1 right

that is the angle between the ND and 100 that is the relation here g 13 is equal to cos of gamma 1 like that the relationship between 010 with RD, TD and ND is cos alpha 2, cos beta 2, cos gamma 2.

On the other hand, the relationship between 001 with respect to RD, TD and ND is cos alpha 3, cos beta 3 and cos gamma 3 right. So, g is an orientation matrix consists of nine variables g 11, g 12, g 13, g 21, g 22, g 23, g 31, g 32, g 33 that is the angle the cosine of the angle between the crystal coordinate systems and the sample coordinate system and that is we have the here in the horizontal the 100 axis is constant. For the first, where I am pointing out in the second one 010 is constantly related with RD, TD and ND; in the third one 001 is related to RD, TD and ND. So, here 100 is related to RD, TD and ND and the rest as I said so.

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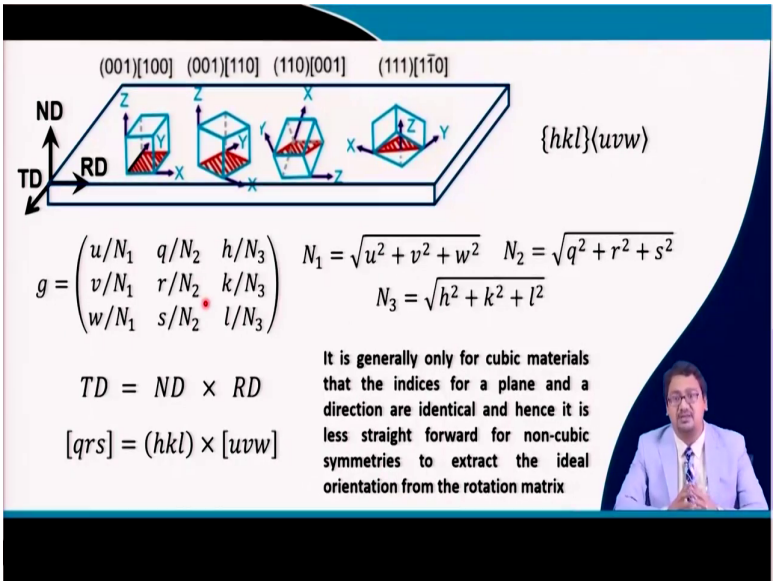

So, if we look closely into the orientation matrix that is the g matrix we can find out that if there is a sample consist of many orientations or few orientations or like this four kind of orientation. Then each of these orientation will have a orientation matrix right and then each of these orientation as because as I said that g did which is cos alpha 1, cos beta 1, cos gamma 1 is the relationship between 100 with RD, TD and ND and like that 010 with RD, TD and ND 001 with RD, TD and ND.

The g matrix can be written in terms of u v and w divided by N 1, where N 1 is root square of u square plus v square plus w square and this u v and w is the miller indices of the RD

right. Whereas qrs divided by q r s, q divided by root square of q square plus r square plus s square r divided by q square root of q square plus r square plus s square s divided by root of q square plus r square plus s square is the cos alpha cos beta 1 cos beta 2 cos beta 3 that is the relationship of g 100, 010, 001 with TD right.

So, this gives the miller indices of TD. Whereas, hkl is the relationship of 100, 010, 001 with ND. So, from the cos alpha 1, beta 1, gamma 1, alpha 2, beta 2, gamma 2, alpha 3, beta 3, gamma 3 one can decipher the hkl, uvw pertaining and qrs pertaining to ND RD and TD. And one can cross check this whether this relation is coming correct by TD is equal to ND cross RD and so, the qrs here must match the qrs by doing the cross product of it. So, that here I will give you a disclaimer that it is generally only for the cubic materials that the indices of the planes and the directions are identical.

So, in case of other material like hexagonal crystal system or trigonal system the planes and the direction are the planes and the perpendicular directions are not identical right. Hence, it is less straightforward in case of non-cubic materials which means that is with non-cubic symmetries to extract the ideal orientation from the orientation matrix like we have done it here and this is only for the cubic crystals. So, one should remember that this relationship of the orientation matrix with the hkl, uvw and qrs that is the important sample reference direction in terms of crystal orientation is for the cubic system and for the non cubic system it becomes a little complex.

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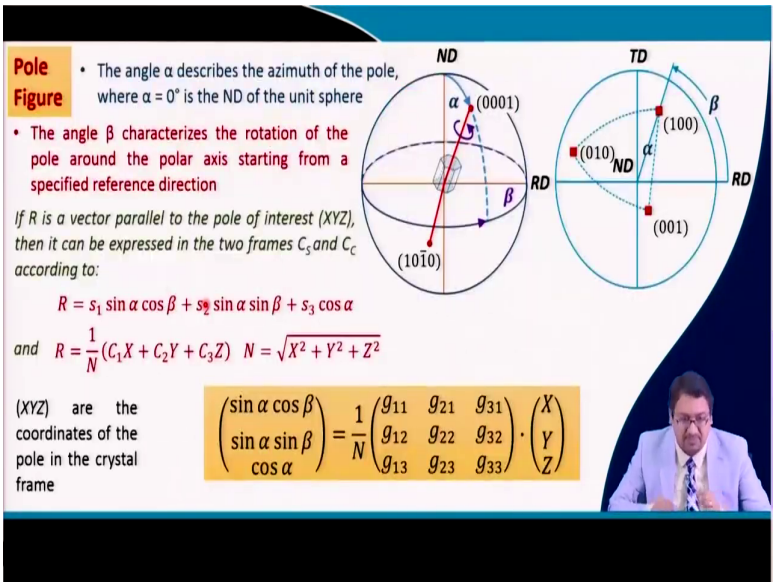

So, finally, if we relate if we try to relate the pole figure which is which we have shown is one way of measuring texture with respect to the orientation matrix and there has to be a relationship because a texture when calculated from a certain processed material. The texture shown in terms of pole figure or in terms of inverse pole figure should match with the miller indices and it should be equal to the orientation matrix. So, what is the mathematical relationship between the pole figure and the orientation matrix; this has to be known right. So, if we talk about the pole figure.

In addition, if we look into this figure this is a three dimensional sphere which has been shown and this is the stereographic projections two dimension of this, three dimension sphere. So, that if we have shown this by a hexagonal unit cell because it is easier to distinguish between different planes when we look into the hexagonal unit cell and say for example, the hexagonal unit cell has an important axis which is the c axis say this is R and this R is at an angle alpha right from the important pole which is the ND and sometimes it is also called the North Pole.

So, if it is at an angle alpha from the North Pole and this is this alpha is described as an azimuth of the pole. So, at ND or at the North Pole alpha is 0 for this units were right and say that the angle beta the angle beta is the rotation of this pole about the RD and which is this one.

So, the angle beta a characterizes the rotation of the pole around this a North Pole which is the polar axis starting from the specified reference direction that is an important reference direction which is RD. So, RD is the most important reference direction and the angle beta can be given by this. This can be also shown for a cubic crystal and this has been shown when we are looking to the stereographic projection from ND; and if we are look looking from ND then that there is an important pole which is this one 100; any one of these three 100 and which is at an angle alpha from ND and then it is about a beta rotated from the important sample reference direction RD.

If r is a vector parallel to the pole of interest like this is 001 0001 and this is 100 that is some plane say XYZ plane or XYZ pole. Then it can be expressed in terms of two frames of references; that is the sample frame of reference which is C s and the crystal frame of reference which is C c right. So, let us express this R in terms of sample frame of reference. So, R is equal to s 1 right. Let us say, this is s 1 and s 1 times this is alpha. So, this is sin of

alpha which comes out to be here and then cos of beta which comes out to be here. So, in terms of s 1 we have described R n plus s 2 which is between the transverse direction some transverse direction here right TD which is 90 degrees to RD and ND.

So, it will be sin of alpha and then it will be sin of beta right. Now, if this is sin of beta then plus s 3 which is with ND and that is s 3 cos of alpha. So, R is equal to s 1 sin alpha cos beta plus s 2 sin alpha sin beta plus s 3 cos alpha that is in terms of the sample reference system. And in terms of the crystal reference system it is 1 by root of the XYZ that is the miller indices of that pole that is the root of X squared plus Y squared plus Z squared times C 1 X plus C 2 Y plus C 3 Z right. So, the crystal coordinate system C 1, C 2 and C 3 with respect to X, Y and Z which is the miller indices for the particular pole of interest with respect to this RD, ND and TD now if. The XYZ is the coordinate of the pole of the crystal frame ok. Now if we relate this sample reference system with the crystal reference system we find out that sin alpha cos beta, sin alpha cos beta, sin alpha sin beta, cos alpha is equal to this is the sample reference system times the g matrix is equal to the a crystal reference system that is XYZ; and normalized crystal reference a crystal reference system that is 1 by N which is root of X square plus Y square plus Z square.

So, C s is times g is equal to C c. Now, if we are writing this then it becomes sin alpha cos beta sin alpha sin beta cos alpha this is the C s; that is a sample reference system equal to the C c which is 1 by N, X Y and Z; g of inverse right. So, it is orientation matrices inverse, inverse of the orientation matrix. This becomes g 11, g 21, g 31, g 12, g 22, g 32, g 13, g 23, g 33. So, the orientation matrix is here in inverse.

Therefore, instead of g 11, g 12 like this it is g 11, g 12, g 13. So, just to remind remember this. So, that we have shown that using the orientation matrix 1 can relate the pole figure the important pole and its angular direction with respect to the important sample reference system with respect to the g matrix which is the orientation matrix. So, pole figures and orientation matrices are mathematically related.

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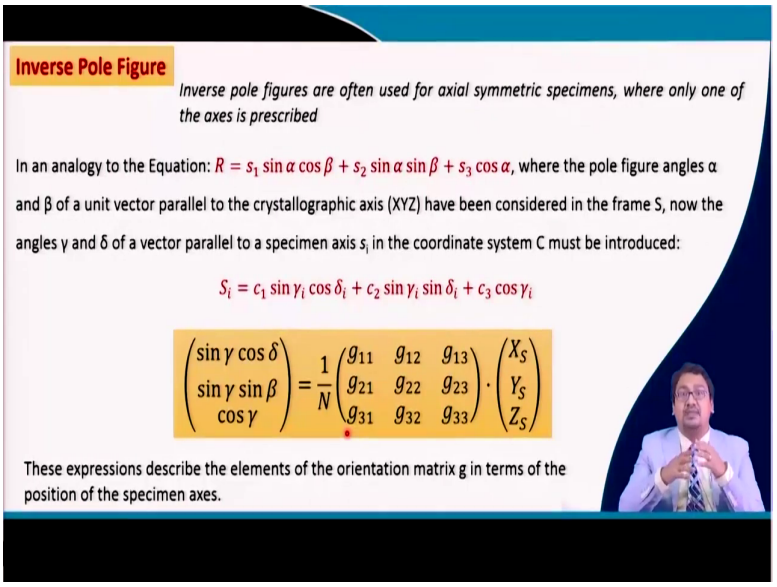

Now, if we look into the inverse pole figure and as we know that inverse pole figure is an important method to show texture and irrespect. And in the pole figure, we represent the crystal direction with respect to the sample direction in the inverse pole figure we represent the sample important sample direction with respect to the crystal direction using one of the triangles from the stereographic projection using the symmetry of the crystal.

So, most of the time inverse pole figure are often used when the sample is actually symmetric and where only one axes is means most important. If we use the analogy of this equation R equal to sin s 1 sin alpha cos beta plus s 2 sin alpha sin beta plus s 3 cos alpha where the for the pole figure, where alpha and beta are the angles between the unit vector XYZ, which is the crystallographic axes in terms of the sample frame of reference. And in this case in case of the inverse pole figure one can use two values of angles gamma and delta in a similar manner for the vector of the specimen axis s 1 in the with respect to a crystal coordinate system C. So instead of R S the important sample reference direction the first one may be say the rolling plane or the rolling direction or in case of extrusion the one singular axis is the extrusion axis.

So, say. So, S i is equal to c 1 which is the first important crystal direction times sin gamma cos delta plus c 2 sin gamma sin delta same as this equation and c 3 cos gamma right. So, in this case also the relationship of this crystal coordinate system in case of pole figure this was the sample coordinate system. The relationship of this crystal coordinate system which is sin

gamma cos delta sin gamma sin sorry it is delta and cos gamma is equal to the sample reference system X Y and Z. X s Y s and Z s normalized by 1 by N whereas, N is equal to root of X s square plus Y s square plus Z s square is in relationship with g here. So, C is equal to C s times g which is g 11, g 12, g 13, g 21, g 22, g 23, g 31, g 32, g 33. So, g 11 is cos alpha 1, g 12 is cos beta 1, g 13 is cos gamma 1 and like this cos of alpha 2 cos of beta 2 cos of gamma 2 cos of alpha 3 cos of beta 3 cos of gamma 3 that is the geometrics is related. These expressions for the pole figure and the inverse pole figure describes the elements of the orientation matrix g in terms of position of the specimen axes and for the inverse pole figure and in terms of the crystal coordinate system in case of the pole figure.

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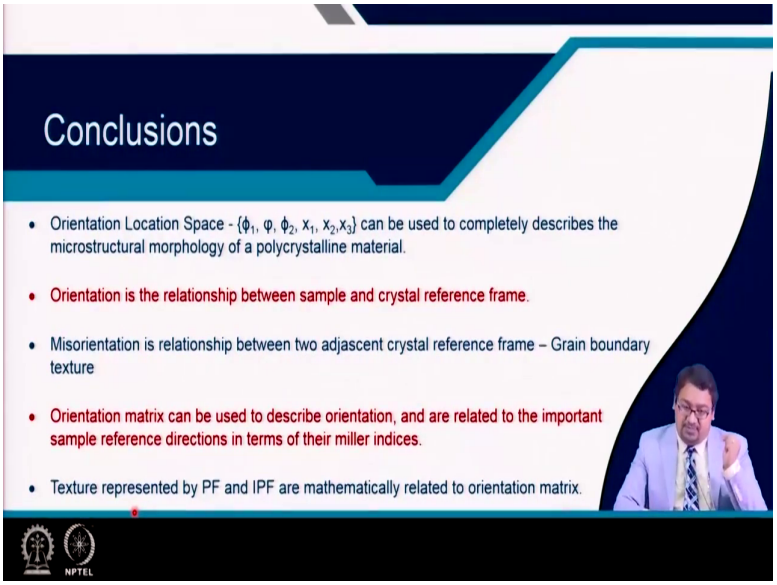

So, from this lecture we can conclude that first orientation location space which is phi 1, phi, phi 2, x 1, x 2, x 3 can be use to completely describe the microstructural morphology of a polycrystalline material orientation. Second orientation is the relationship between the sample and the crystal frame of reference. Misorientation is the relationship between two adjacent crystal frame and misorientation gives the grain boundary texture right.

If we have two grains adjacent grains with two different orientation the mismatch between the orientation gives delta g which is known as misorientation and is also a form of texture and is known as grain boundary texture misorientation matrix is can be used to describe the orientation. So, g matrix can be used it has nine variables and so, it is it can be used to describe the orientation and are related to the important sample reference direction in terms of

miller indices we have shown that how g matrices is related to hkl, uvw and qrs of RD, TD and ND important sample reference system. Then, the texture represented by the pole figure and the inverse pole figure are mathematically related to the orientation matrices.

Thank you.