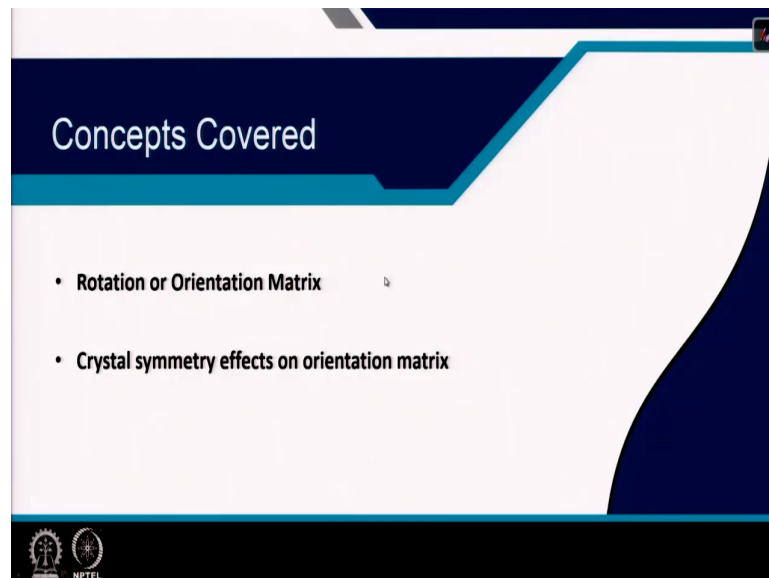


Texture in Materials
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Module - 04
Texture representation
Lecture - 17
Symmetry Effects on Orientation Matrix

Good day everyone. Today we will continue with the module 4, which is texture representation. Today is lecture 17, in which we will show the symmetry effects on orientation matrix. So, let us start.

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Therefore, the concepts that will be covered in this class are rotation or orientation matrix second crystal symmetry effects on orientation matrix.

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Orientation If the crystal and sample coordinate system is known or specified

→ The relative angular position of the crystal coordinate system with respect to the sample coordinate system is known as ORIENTATION " g "

$$C_C = g \cdot C_S$$

' g ' can be expressed as →

Miller indices → Pole Figures → Inverse Pole Figure

Euler Space (ODF) → Angle/axis pair → Rodrigues Space

Fundamental way of expressing g → **Rotation or Orientation Matrix** is the rotation of sample coordinate system onto the crystal coordinates

The slide features a blue header and footer, a white main content area, and a small inset video of a man in a suit in the bottom right corner.

In the previous lectures, we have understood what is an orientation matrix, which is also known as rotation matrix right. So, a orientation matrix is related to orientation right. So, what is an orientation? Orientation is the relationship between the sample and the crystal coordinate system.

So, if a crystal and the sample coordinate systems are known or is specified then, we can find out the relative angular positions of the crystal coordinate system with respect to the sample coordinate system. This is known as orientation right or a specific texture right a specific texture component, which can be given by g . Usually we show that by g right.

So, the relationship between the crystal coordinate system which is C_C is equal to g , which is the orientation times the sample coordinate system right C_S . So, g , which is the orientation can be expressed in terms of the most basic thing is using Miller indices.

So, we can use miller indices like planes and directions to show it and we have discussed about it earlier in earlier class. And Miller indices is shown by using two tools, specifically in texture and that are pole figures and then the inverse pole figures right.

So, the other way of expressing the g is the Euler angles right. So, we use Euler angles ϕ_1 , ϕ_2 and then, we can plot that in Euler space and show them as orientation distribution functions we call them ODF's right. The another way of expressing g is axis angle pair and

logic space. So, these are the important tools by which we express the orientation that we are obtaining in our experiments right.

So, but the most fundamental way of expressing g is the rotation matrix or the orientation matrix. In addition, what is the rotation or the orientation matrix? It is the rotation of the sample coordinate system into the crystal coordinate system and that we have seen in the previous lectures.

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Rotation or Orientation Matrix

$$g = \begin{matrix} & \begin{matrix} RD & TD & ND \end{matrix} \\ \begin{matrix} \cos \alpha_1 \\ \cos \alpha_2 \\ \cos \alpha_3 \end{matrix} & \begin{pmatrix} \cos \beta_1 & \cos \beta_2 & \cos \beta_3 \\ \cos \gamma_1 & \cos \gamma_2 & \cos \gamma_3 \end{pmatrix} \end{matrix} \begin{matrix} 100 \\ 010 \\ 001 \end{matrix}$$

So, what is it? So, g is equal to the matrix which contains $\cos \alpha_1$, which is the relationship between the sample coordinate system $R D$ that is the rolling direction, with respect to the specimen coordinate system $1 0 0$ sorry the crystal coordinate system $1 0 0$ right.

In this way, when transverse direction is related to the crystal coordinate system $1 0 0$, it becomes $\cos \beta_1$. And like that when the normal direction $N D$ relates the angular relationship with $1 0 0$, it becomes $\cos \gamma_1$. Like that; the $R D$ $T D$ and $N D$ can be related to $0 1 0$ to form $\cos \alpha_2$ $\cos \beta_2$ $\cos \gamma_2$ and with $0 0 1$ to form $\cos \alpha_3$ $\cos \beta_3$ $\cos \gamma_3$ right. So, this is the way that an orientation matrix is defined.


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Rotation or Orientation Matrix

$$g = \begin{pmatrix} \cos \alpha_1 & \cos \beta_1 & \cos \gamma_1 \\ \cos \alpha_2 & \cos \beta_2 & \cos \gamma_2 \\ \cos \alpha_3 & \cos \beta_3 & \cos \gamma_3 \end{pmatrix} = \begin{pmatrix} g_{11} & g_{12} & g_{13} \\ g_{21} & g_{22} & g_{23} \\ g_{31} & g_{32} & g_{33} \end{pmatrix} = \begin{pmatrix} u/N_1 & q/N_2 & h/N_3 \\ v/N_1 & r/N_2 & k/N_3 \\ w/N_1 & s/N_2 & l/N_3 \end{pmatrix}$$

Orientation matrix expresses the important sample reference directions in terms of the crystal directions that are parallel to them.

- Both rows and columns of the rotation matrix are unit vectors
 - Matrix is orthonormal → $g^{-1} = g^T$
- The orientation matrix contains 9 non-independent variables
- Cross product of two rows/columns gives the third
- For any row/column → sum of square = Unity



And the orientation matrix, the $\cos \alpha_1 \cos \beta_1 \cos \gamma_1$. And all the other 9 variables are shown with respect to $g_{11} g_{12} g_{13} g_{21} g_{22} g_{23} g_{31} g_{32} g_{33}$ like this in the matrix. And what are these? And as we have seen that it is the relationship between R D right T D and N D with $1\ 0\ 0\ 0\ 1\ 0\ 0\ 0\ 1$. Then, we have found out that of course, then this g_{11} is $g_{11} g_{21}$ and g_{31} is related to R D.

So, if the Miller indices of R D is $u\ v$ and w then, the $g_{11} g_{21}$ and g_{31} is u divided by root square of $u^2 + v^2 + w^2$, which is given by N_1 right. Like that it is for the g_{21} and it is for the g_{31} . On the other hand, if $h\ k\ l$ is the Miller indices for the N D then, h divided by N_3 , where N_3 is $\sqrt{h^2 + k^2 + l^2}$ is the g_{13} right and like that k by n_3 is g_{23} and l by N_3 is g_{33} right. This is the relationship between the Miller indices and the orientation matrix, which we clearly understand. On the other hand, if we take the middle row middle column sorry and that is $g_{12} g_{22}$ and g_{32} and this is the T D direction. And could be given by $q\ r\ s$ divided by N_2 and where N_2 is equal to $\sqrt{q^2 + r^2 + s^2}$ right.

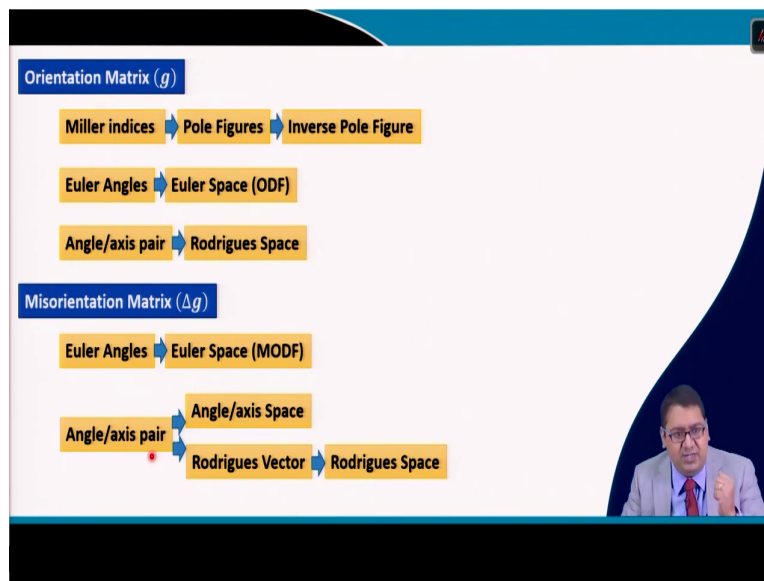
So, the orientation matrix expresses the important sample reference direction, in terms of the crystal direction that are parallel to them; that means, that $u\ v\ w$ are parallel to R D, $q\ r\ s$ is parallel to T D, $h\ k\ l$ is parallel to N D. It represents the important sample reference direction, in terms of the crystal directions that are parallel to them right.

So, if we look closely to the orientation matrix, you can find out that the both the row rows and the columns of this matrix are unit vectors right. Therefore, if you add them, it become if you add the square of them, it becomes unity. So, that this matrix is orthonormal. Therefore, the inverse of the g matrix is equal to the transverse of the g matrix right.

So, moreover, what we understood from this study is that the orientation matrix contains 9 non-independent variable $u v w q r s h k l$ divided by their respective square roots the cross product of two rows. So, cross product of two rows gives the third one right. So, a cross product of $N D$ cross $R D$ gives $T D$, $T D$ cross $N D$ gives $R D$ right $R D$ cross $T D$ gives $N D$ right.

Therefore, you get the third by using the cross product. In addition, for any row or column, the sum of square becomes equal to unity and that is why it its g inverse is equal to g transpose right.

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So, what we understood from here, is that the orientation matrix which is given by g is most of the time expressed in terms of Miller indices in form of pole figures or inverse pole figures. It is expressed in terms of Euler angles in Euler space mostly in form of Orientation Distribution Function O D F. Otherwise; it is expressed in terms of axis angle pair or vertical space.

We have also seen that misorientation matrix; that is delta g, which is a homologous to the orientation matrix. The orientation matrix is the relationship between the sample coordinate system and the crystal coordinate system; whereas, the delta g is the relationship between two crystal coordinate system adjacent crystal coordinate system.

As for example, in a poly crystalline material, if there are presence of different grains, the relationship the misorientation relationship between the two grains may will cause will produce a matrix delta g, which will have the same nine variables like that like in the orientation matrix. Therefore, we can represent that in terms of Euler angle and in terms of Euler space. In this case, it is known as M O D F; that is Misorientation Orientation Distribution Function. In addition, we can show that in terms of axis angle axis pair and we can show it in the angle axis space or in terms of Rodrigues vectors or in the; that means, in the Rodrigues space right.

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Crystallographic related solutions for Orientation Matrix

Orientation matrix is the relationship between crystal and sample coordinate system.

Number of solutions may exist and will depend on the crystal and sample symmetry.

Considering Crystal symmetry for cubic crystals

Eg. $(12\bar{3})[634]$

$$g = \begin{pmatrix} \cos \alpha_1 & \cos \beta_1 & \cos \gamma_1 \\ \cos \alpha_2 & \cos \beta_2 & \cos \gamma_2 \\ \cos \alpha_3 & \cos \beta_3 & \cos \gamma_3 \end{pmatrix} = \begin{pmatrix} g_{11} & g_{12} & g_{13} \\ g_{21} & g_{22} & g_{23} \\ g_{31} & g_{32} & g_{33} \end{pmatrix} = \begin{pmatrix} u/N_1 & q/N_2 & h/N_3 \\ v/N_1 & r/N_2 & k/N_3 \\ w/N_1 & s/N_2 & l/N_3 \end{pmatrix}$$

$$= \begin{pmatrix} 6/\sqrt{61} & 17/\sqrt{854} & 1/\sqrt{14} \\ 3/\sqrt{61} & 22/\sqrt{854} & 2/\sqrt{14} \\ 4/\sqrt{61} & -9/\sqrt{854} & -3/\sqrt{14} \end{pmatrix}$$

So, . So, based upon the crystallography; that means, the crystal structure and the crystal symmetry, there could be many related solutions for a single orientation matrix; that means, there could be a number of orientation matrix there could be a number of solutions right. So, the orientation matrix depends upon the angular relationship between the crystal and the sample coordinate system.

A number of solutions may exist, because there are crystal symmetry and sample symmetry. In addition, what do you mean by crystal symmetry? Because the crystal has point group or

space group symmetry. Therefore, mainly here, we are talking about the point group symmetry; that is the rotational symmetry and the sample symmetry. The sample symmetry depends upon the type of process that the sample has undergone.

Therefore, whether it is a rolling or a particular kind of a casting so, each will lead to have a certain kind of symmetry or no symmetry in the sample. Thus, the requirement of symmetry is the understanding of the symmetry crystal symmetry and the sample symmetry is required to understand that there could be many solutions that may exist to show a particular orientation. And that means, there could be number of orientation matrices, based upon the crystal and the sample symmetry which show the same orientation. So, let us start with a nice example, considering the crystal symmetry for cubic crystals. Example is the ND plane is $1\ 2\ \bar{3}$ and the RD is $6\ 3\ 4$. So, that, if we take this example and we try to draw the orientation matrix g relating $1\ 2\ \bar{3}\ 6\ 3\ 4$ with RD, TD and ND whereas, $1\ 2\ \bar{3}$ is ND and $6\ 3\ 4$ is RD.

Therefore, that $u\ v\ w$ divided by $N\ 1$. The $N\ 1$ is roots root over $6\ \text{square} + 3\ \text{square} + 4\ \text{square}$ which comes out to be 61. So, root over 61 and. So, $6\ 3\ 4$ divided by root over 61 gives the first column of the g matrix. The third column of the g matrix which indicates ND is given by $1\ 2$ and minus 3 divided by $1\ \text{square} + 2\ \text{square} + 3\ \text{square}$ root over. Therefore, which comes to be equal to be 14 right. So, we do the cross product of ND and RD and we can find out the value of TD which comes out to be $17\ \text{root over } 854\ 22\ \text{root over } 8\ \text{over } 52\ 9\ \text{divided by root over } 854$ right. Therefore, this is the orientation matrix corresponding to the Miller indices that is the texture $1\ 2\ \bar{3}\ 6\ 3\ 4$ right. So, $1\ 2\ \bar{3}$ is ND $6\ 3\ 4$ is RD.

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Effect of crystal symmetry on Orientation Matrix

Depending on crystal and sample symmetry a number of solutions of 'g' may exist simultaneously

Considering Cubic Crystal → There are 24 different ways the crystal with cubic symmetry can be arranged

→ There are 24 crystallographically related solutions for an orientation matrix

4 - $\langle 111 \rangle$ → 3 fold symmetry → 2 rotations of 120° about 4 $\langle 111 \rangle$ axes,
 3 - $\langle 100 \rangle$ → 4 fold symmetry → 3 rotations of 90° about 3 $\langle 100 \rangle$ axes,
 6 - $\langle 110 \rangle$ → 2 fold symmetry → 1 rotations of 180° about 6 $\langle 110 \rangle$ axes,
 and the Identity matrix

NOTE: There are 12 and 4 solutions for an orientation matrix of materials having hexagonal and orthorhombic symmetry respectively.

So, that I have said that depending upon the crystal and the sample symmetry, a number of solutions of the g matrix can exist simultaneously right. So, let us consider the cubic crystal.

Now, cubic crystal if you look that there are 24 different ways the crystals of the cubic symmetry can be arranged. Now, this can be find out even from the stereographic projection. So, if you look into the standard 1 0 0 stereographic projection and that the stereographic projections are is, divided into number of triangles with corners 1 0 0, 0 1 1, 1 1 1. In addition, there are num number of triangles having the same corner 0 0 1 bar 1 0 1 bar 1 1 bar 1 bar. So, each of them consisting of the family of poles for the family of planes 1 0 0, 1 1 0 and 1 1 1.

So, that if you look in this quadrant of the stereographic projection, you can see 1 2 3 4 5 and 6 triangles like this. So, if we multiply this 6 into this 3 into this 4-quadrant then, 6 into 4 is 24 right. Therefore, there are 24 different ways the particular orientation or a particular texture component could be observed in the stereographic projection.

Now, there is a different way to understand this thing. So, if that what are the 24 crystallographically related solutions for the orientation matrix. You can see that it has 4 - 1 1 1 axis which has 3 - fold symmetry right. So, if we give two rotations by 120 degrees about the 4 - 1 1 1 axis it goes to the new position, but the crystal looks exactly the same right. On the other hand, it has 3 - 1 1 0 axis with 4-fold symmetries.

So, if that if we give along a 1 0 0 axis ok. If you give a rotation by 90 degree, it comes exactly to the same. It looks that it has not been rotated right like that, you can give 90, 90, 90 rotation and it will be always look likes the same.

Similarly, it has 6- 1 1 0 axis with 2-fold symmetry. So, if you give one rotation of 180 degree along any of the 1 0 0 axis any of the 6- 1 0 0 axis, it comes to the same position. So, and there is the position where there is no rotation; that is the identity matrix right. So that if we add like the first one; that is the 4 into 2 that is 8 and then, 3 into 3 for the 1 0 0 axis that is 9. So, 8 plus 9 is 17 and 6 into 1; that means, 17 plus 6 is 23 plus the identity matrix becomes 24. So, there are 24 crystallographically related solution for the cubic crystals, because of this kind of symmetry element which is point group symmetry which is present in it.

So, well ok so, if you note that. There are 12 and 4 solutions for the orientation matrix for material having hexagonal. So, there are 12 solution for the hexagonal system hexagonal close packed system and 4 for the orthorhombic symmetry systems right. Similar and the similar solutions can be obtained by observing the similar kind of explanation.

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The 24 crystallographic solution for $(12\bar{3})[634]$

These different miller indices represents different matrices

Each of these matrices describe same orientation

Each of these matrices hold a different position in Euler Space

are:

$$g = \begin{pmatrix} 6/\sqrt{61} & 17/\sqrt{854} & 1/\sqrt{14} \\ 3/\sqrt{61} & 22/\sqrt{854} & 2/\sqrt{14} \\ 4/\sqrt{61} & -9/\sqrt{854} & -3/\sqrt{14} \end{pmatrix}$$

$(123)[634]$	$(\bar{1}23)[\bar{6}34]$	$(1\bar{2}3)[6\bar{3}4]$	$(12\bar{3})[634]$
$(132)[643]$	$(\bar{1}32)[\bar{6}43]$	$(13\bar{2})[643]$	$(1\bar{3}2)[\bar{6}43]$
$(213)[364]$	$(\bar{2}13)[\bar{3}64]$	$(21\bar{3})[364]$	$(2\bar{1}3)[\bar{3}64]$
$(231)[346]$	$(\bar{2}31)[\bar{3}46]$	$(23\bar{1})[346]$	$(2\bar{3}1)[\bar{3}46]$
$(312)[463]$	$(\bar{3}12)[\bar{4}63]$	$(31\bar{2})[463]$	$(3\bar{1}2)[\bar{4}63]$
$(321)[436]$	$(\bar{3}21)[\bar{4}36]$	$(32\bar{1})[436]$	$(3\bar{2}1)[\bar{4}36]$

$$\begin{pmatrix} 3/\sqrt{61} & 22/\sqrt{854} & 2/\sqrt{14} \\ 6/\sqrt{61} & -17/\sqrt{854} & 1/\sqrt{14} \\ 4/\sqrt{61} & 9/\sqrt{854} & -3/\sqrt{14} \end{pmatrix}$$

$$\begin{pmatrix} -3/\sqrt{61} & 22/\sqrt{854} & -2/\sqrt{14} \\ -4/\sqrt{61} & -9/\sqrt{854} & 3/\sqrt{14} \\ 6/\sqrt{61} & 17/\sqrt{854} & 1/\sqrt{14} \end{pmatrix}$$

$$\begin{pmatrix} 6/\sqrt{61} & -17/\sqrt{854} & 1/\sqrt{14} \\ 3/\sqrt{61} & -22/\sqrt{854} & 2/\sqrt{14} \\ -4/\sqrt{61} & 9/\sqrt{854} & 3/\sqrt{14} \end{pmatrix}$$

So, that let us go to this cubic crystal and see that for the 1 2 3 bar 6 3 4 kind of texture, how 24 different crystallographic solutions can exist right. So, let us go. So, that if we look into the family of planes for the 1 2 3 right, there could be 1 2 3 bar type plane right, which is this one. And there could be 1 2 bar 3 and there could be 1 bar 2 3, there could be 1 2 3.

And these all four planes are different planes and related to which the direction which is $R D$ $6\ 3\ 4$, which is for this particular. The combination could be determined, because the $R D$ lies in the $N D$ plane right. So, let us say there are four combinations that can be determined right. Now, for each combination. Let us talk about this one; $1\ 2\ 3$, $6\ 3\ 4$ bar, we can find out by changing the position from $1\ 2\ 3$ to $1\ 3\ 2$ to $2\ 1\ 3$, $2\ 3\ 1$, $3\ 1\ 2$, $3\ 2\ 1$ like this.


By changing the position, we can find out the values of $R D$, which will also change positions accordingly. Therefore, there are how many solutions. There are six solutions like this for this particular by changing the positions of the Miller indices. Then, like that, we can do it for all the four of them. Therefore, you can see that there are 24 crystallographic solution for the same texture same orientation. Now, for each one of them, there will be a different the orientation matrix. So, for $1\ 2\ 3$, $6\ 3\ 4$ bar, it is $6\ 3$ minus 4 , $1\ 2\ 3$ of course, divided by the root mean square of their value right.

Then, the $T D$ is minus 17 minus $22\ 9$ divided by root of 854 . If we take another one. Of course, which is this one. there is a subtle change here, 6 divided by divided by root of $61\ 3$ and 4 right. On the other hand, $1\ 2$ and minus 3 . It will happen like this, because the position of the Miller indices are changing accordingly for each of this 24 cases right. If we look into the case, it shows the orientation matrix slightly different from the other one. Therefore, each one of this (hkl) $[uvw]$ texture will have a different Miller indices. Here, is another example. We have given four examples and one can find out for each one of these 24 cases different orientation matrices right. So that there is subtle differences in the sign and the positions and therefore, each orientation matrix is different. This shows that these different Miller indices representing different matrices contains or show the same orientation right. Now, each of these matrices holds a different position in the Euler space.

So, when we are looking into the Euler space or Orientation Distribution Function or $O D F$'s, we will find that for each of these Miller indices or each of this orientation matrices, there will be a different ϕ_1 , ϕ_2 in the Euler space. And all those components in the Euler space seem will be seems to be repeated many times, but it will represent the same orientation and this occurs, because of the symmetry of the cubic crystal.

And it will occur the same for the hexagonal and the orthonormal sorry orthogonal symmetry systems. But in for hexagonal, it will be 12 crystallographic solution. For orthogonal, it will be only 4 crystallographic solutions.

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Conclusions

- Orientation matrices are the most fundamental means of expressing an orientation or texture component.
- There are 24 solutions for orientation matrix in cubic crystals.
- There are 12 solutions for orientation matrix in hexagonal crystals.
- There are 4 solutions for orientation matrix in orthorhombic crystals

The conclusions are that orientation matrices are the most fundamental means of expressing the orientation or the texture components right. These orientation matrices could be related to the Miller indices via the pole figure or the inverse pole figures right. It could be related to the Euler angles via the Euler space and the Orientation Distribution Functions O D F's. It could be related to the angle axis pair through Rodrigues vectors or Rodrigues space right.

There are 24 solutions for orientation matrices in cubic crystals right. There are 12 solutions for orientation matrix, in case of hexagonal crystals with hexagonal symmetry and there are 4 solutions for orientation matrix in case of orthorhombic symmetries.

Thank you very much.