

Crystallographic orientation representations

- Euler Angles
- Axis-Angle
- Rodrigues-Frank Vectors
- Unit Quaternions

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27-750

Texture, Microstructure & Anisotropy

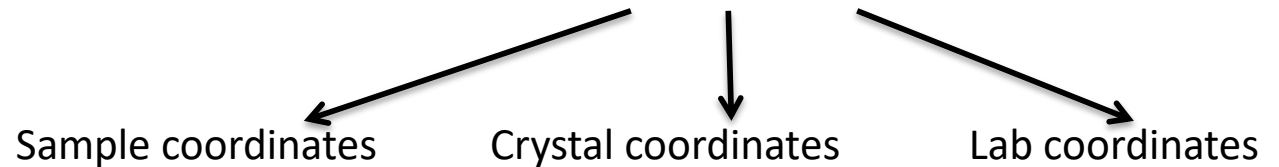
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Lecture Objectives

- Brief review on the challenges of describing crystallographic orientations
- Review of previously studied orientation representations: rotation matrices and Euler angles
- Introduction of Rodrigues-Frank vectors
- Introduction of unit quaternions
- Useful math for using quaternions as rotation operators
- Conversions between Euler angles, axis-angle pairs, RF vectors, and quaternions

Why can it be challenging to work with crystallographic orientations?

- Orientation is specified based on reference frames

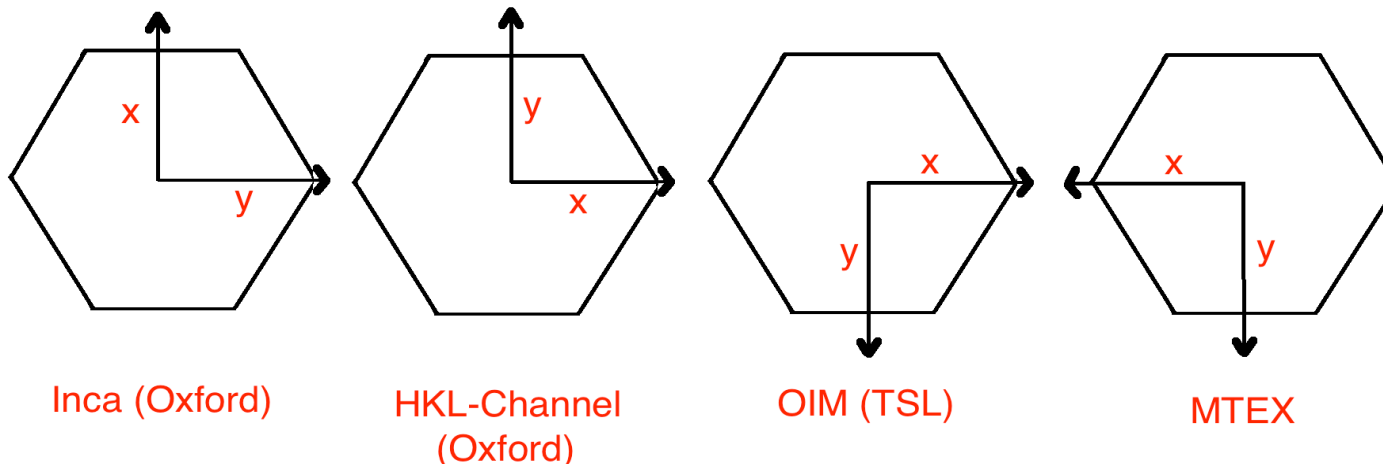


- Different choices of axes to convert crystal frames

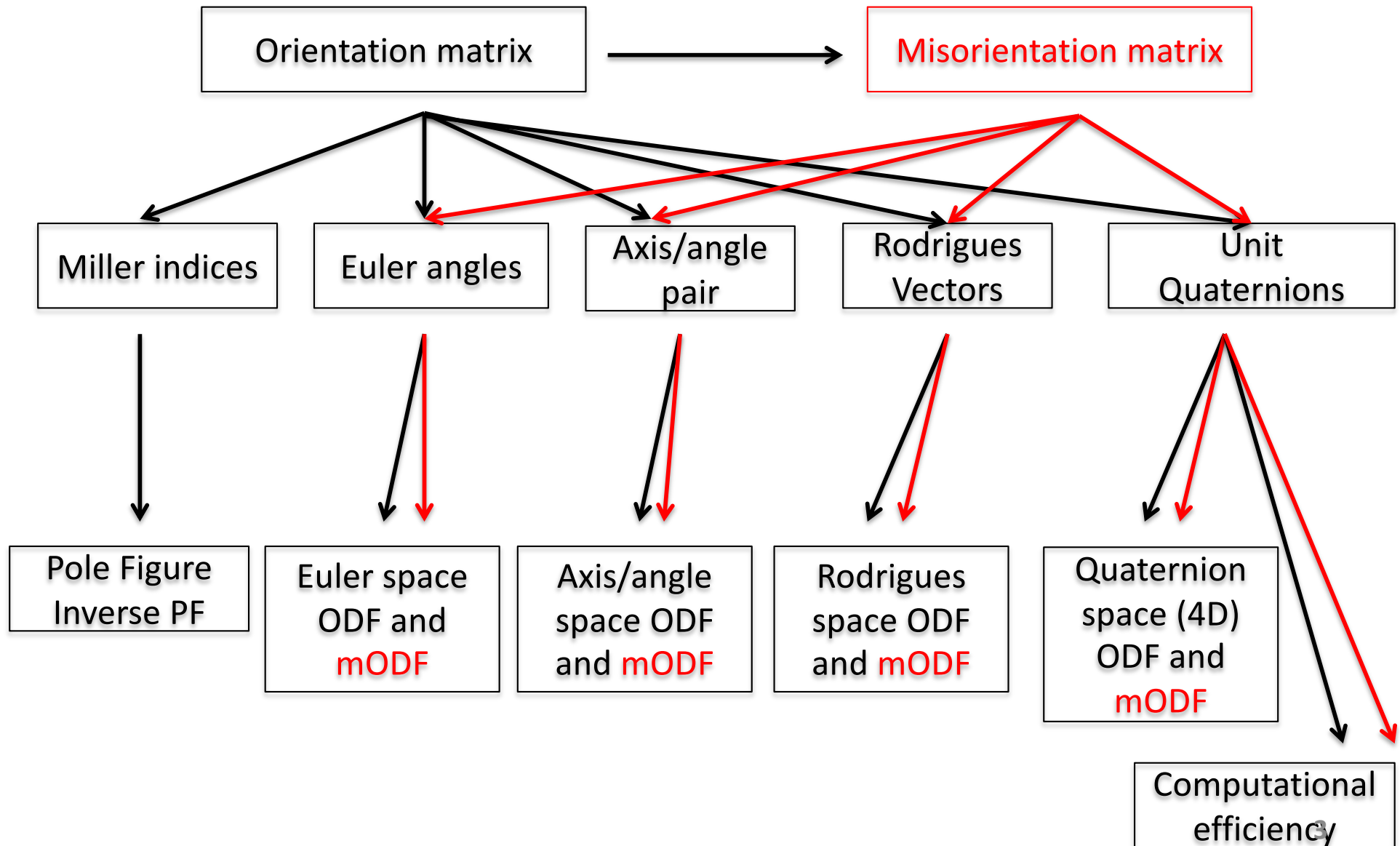
- Hexagonal frame into orthonormal frame

– $x=[10\bar{1}0]$ $y=[\bar{1}2\bar{1}0]$ $z=[0001]$ or $x=[2\bar{1}\bar{1}0]$ $y=[01\bar{1}0]$ $z=[0001]$

- Personal experiences?



Descriptors of orientation



Crystal Orientation: Rotation (direction cosine) Matrices

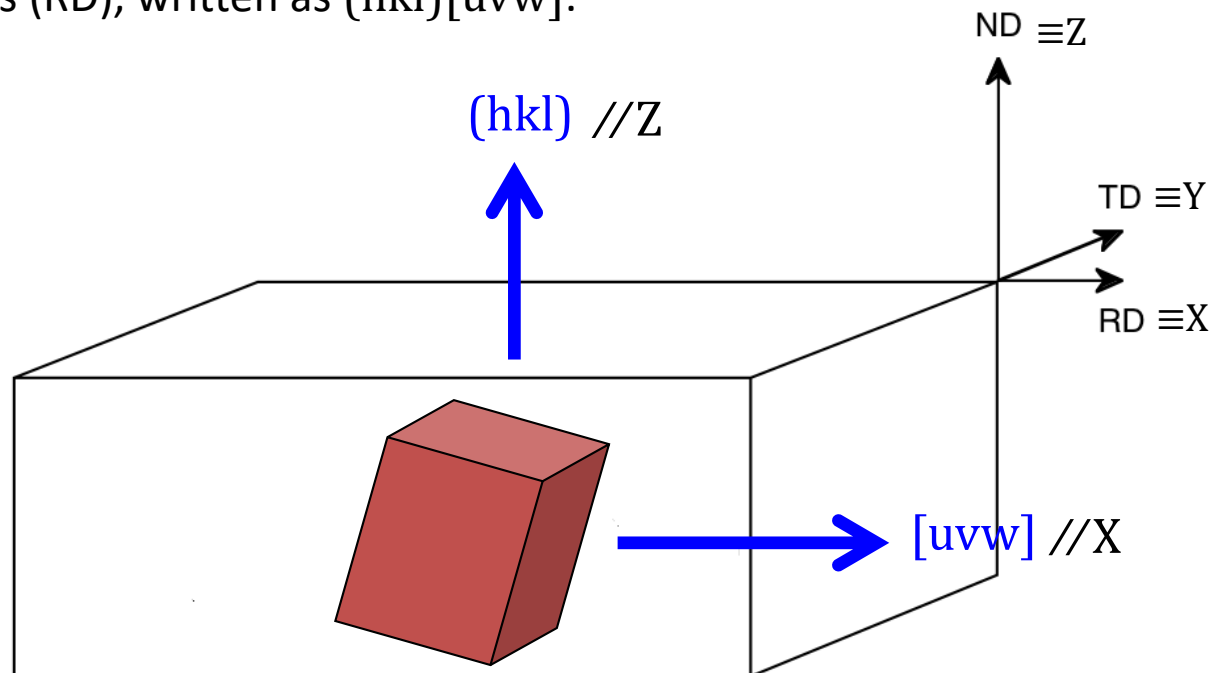
- Crystallographic orientation is the position of crystal system with respect to the specimen coordinate system.
- A single rotation can be described by a rotation axis and an angular offset about the axis.
 - **Passive rotation:** Rotation of axes, sample coordinate into crystal coordinate and *vice versa*.
 - Active rotation: Rotation of the object, crystal coordinate into sample coordinate.

$$R = \begin{pmatrix} \cos \theta & \sin \theta \\ -\sin \theta & \cos \theta \end{pmatrix} \quad \text{vs.} \quad R = \begin{pmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{pmatrix}$$

- 3x3 rotation matrices, R, left-multiply column vectors
- Properties:
 - $R^{-1} = R^T$ and $\det(R) = 1$
 - Rows and columns are unit vectors, and the cross product of two rows or columns gives the third.

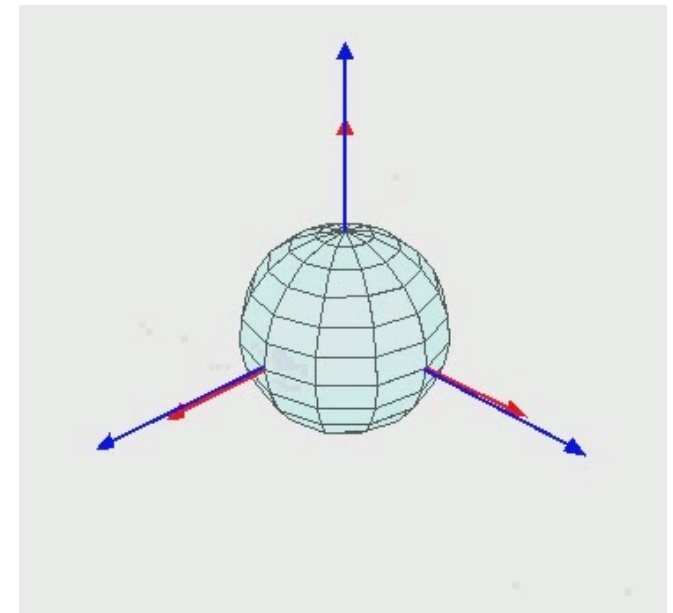
Crystal Orientation: Miller Indices Notation

- Three orthogonal directions chosen as the reference frame
- All directions can then be described as linear combinations of the three unit direction vectors.
- Most straightforward in orthonormal systems, *e.g.*, cubic, as indices for plane and direction are identical.
- In many cases we use the metallurgical names Rolling Direction (RD) // x , Transverse Direction (TD) // y , and Normal Direction (ND) // z .
- We then identify a plane normal parallel to 3rd axis (ND) and a crystal direction parallel to the 1st axis (RD), written as $(hkl)[uvw]$.



Crystal Orientation: Euler Angles

- Euler showed three sequential rotations about different axes can describe orientations (18th century)
- Passive rotation (SCoord into CCoord)
- There are 12 different possible axis-angle sequences.
- The “standard” sequence varies from field to field.
- Multiple conventions
 - **Proper Euler angles** (z-x-z, x-y-x, y-z-y, z-y-z, x-z-x, y-x-y)
 - **Tait–Bryan angles** (x-y-z, y-z-x, z-x-y, x-z-y, z-y-x, y-x-z)
- We use the Bunge convention.
 - First angle ϕ_1 about ND
 - Second angle Φ about new RD
 - Third angle ϕ_2 about newest ND
- Sample symmetry effects the size of Euler space
 - Most general, triclinic crystal system, no sample symmetry $\rightarrow 0 \leq \phi_1, \phi_2 \leq 360 \quad 0 \leq \Phi \leq 180$
 - Cubic crystal system, rolled sample (orthonormal sample symmetry) $\rightarrow 0 \leq \phi_1, \phi_2 \leq 90 \quad \Phi \leq 90$



Rotation matrices from Miller indices

	$[uvw] \equiv \text{RD}$	TD	$ND \equiv (hkl)$	
	↓	↓	↓	
[100] direction →	$\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix}$			Rows are the direction cosines for [100], [010], and [001] in the sample coordinate system, columns are the direction cosines (i.e. hkl or uvw) for the RD, TD and ND in the crystal coordinate system.
[010] direction →				
[001] direction →				

$$\hat{\mathbf{n}} = \frac{(h, k, l)}{\sqrt{h^2 + k^2 + l^2}}$$

$$\hat{\mathbf{b}} = \frac{(u, v, w)}{\sqrt{u^2 + v^2 + w^2}}$$

$$\hat{\mathbf{t}} = \frac{\hat{\mathbf{n}} \times \hat{\mathbf{b}}}{|\hat{\mathbf{n}} \times \hat{\mathbf{b}}|}$$

$$a_{ij} = \text{Crystal} \begin{pmatrix} b_1 & t_1 & n_1 \\ b_2 & t_2 & n_2 \\ b_3 & t_3 & n_3 \end{pmatrix} \text{Sample}$$

Challenge: With Miller indices, we define the closest family (can be degrees away)

Rotation matrices from Bunge Euler angles

$$Z_1 = \begin{pmatrix} \cos \phi_1 & \sin \phi_1 & 0 \\ -\sin \phi_1 & \cos \phi_1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad X = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos \Phi & \sin \Phi \\ 0 & -\sin \Phi & \cos \Phi \end{pmatrix}, \quad Z_2 = \begin{pmatrix} \cos \phi_2 & \sin \phi_2 & 0 \\ -\sin \phi_2 & \cos \phi_2 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Combine the 3 rotations via matrix multiplication; 1st on the right, last on the left:

$$A = Z_2 X Z_1 = \begin{matrix} & \begin{matrix} [uvw] \end{matrix} & & \begin{matrix} (hkl) \end{matrix} \\ \begin{pmatrix} \cos \varphi_1 \cos \varphi_2 & \sin \varphi_1 \cos \varphi_2 & \sin \varphi_2 \sin \Phi \\ -\sin \varphi_1 \sin \varphi_2 \cos \Phi & +\cos \varphi_1 \sin \varphi_2 \cos \Phi & \sin \varphi_2 \sin \Phi \\ -\cos \varphi_1 \sin \varphi_2 & -\sin \varphi_1 \sin \varphi_2 & \cos \varphi_2 \sin \Phi \\ -\sin \varphi_1 \cos \varphi_2 \cos \Phi & +\cos \varphi_1 \cos \varphi_2 \cos \Phi & \cos \varphi_2 \sin \Phi \\ \sin \varphi_1 \sin \Phi & -\cos \varphi_1 \sin \Phi & \cos \Phi \end{pmatrix} \end{matrix}$$

Miller indices from Bunge Euler angles

- Compare the indices matrix from slide 6 with the Euler angle matrix from slide 8.

$$h = n \sin \Phi \sin \varphi_2$$

$$k = n \sin \Phi \cos \varphi_2$$

$$l = n \cos \Phi$$

$$u = n' (\cos \varphi_1 \cos \varphi_2 - \sin \varphi_1 \sin \varphi_2 \cos \Phi)$$

$$v = n' (-\cos \varphi_1 \sin \varphi_2 - \sin \varphi_1 \cos \varphi_2 \cos \Phi)$$

$$w = n' \sin \Phi \sin \varphi_1$$

$n, n' =$ factors to make integers towards the closest family

Bunge Euler angles from rotation matrices

Notes:

The range of inverse cosine (ACOS) is $0-\pi$, which is sufficient for Φ ;

from this, $\sin(\Phi)$ can be obtained;

The range of inverse tangent is $0-2\pi$, (must use the ATAN2 function) which is required for calculating ϕ_1 and ϕ_2 .

$$\Phi = \cos^{-1}(a_{33})$$
$$\varphi_2 = \tan^{-1}\left(\frac{(a_{13}/\sin\Phi)}{(a_{23}/\sin\Phi)}\right)$$
$$\varphi_1 = \tan^{-1}\left(\frac{(a_{31}/\sin\Phi)}{(-a_{32}/\sin\Phi)}\right)$$

$$\text{if } a_{33} \approx 1, \Phi = 0, \varphi_1 = \frac{\tan^{-1}\left(\frac{a_{12}}{a_{11}}\right)}{2}, \text{ and } \varphi_2 = -\varphi_1$$

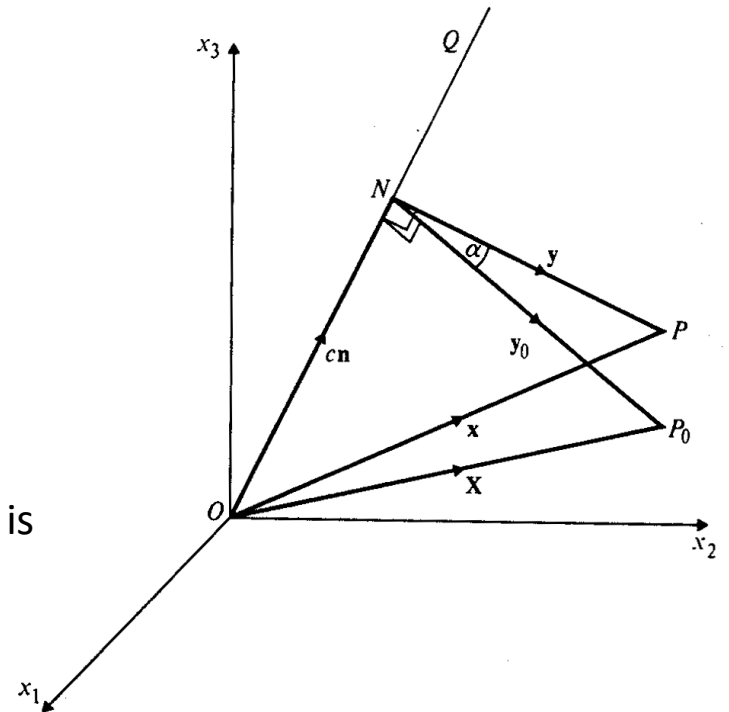
Bunge Euler angles from miller indices

$$\begin{aligned}\cos \Phi &= \frac{l}{\sqrt{h^2 + k^2 + l^2}} \\ \cos \varphi_2 &= \frac{k}{\sqrt{h^2 + k^2}} \\ \sin \varphi_1 &= \frac{w}{\sqrt{u^2 + v^2 + w^2}} \frac{\sqrt{h^2 + k^2 + l^2}}{\sqrt{h^2 + k^2}}\end{aligned}$$

Caution: when one uses the inverse trig functions, the range of result is limited to $0^\circ \leq \cos^{-1} \theta \leq 180^\circ$, or $-90^\circ \leq \sin^{-1} \theta \leq 90^\circ$. Thus, it is not possible to access the full 0-360° range of the angles. It is more reliable to go from Miller indices to an orientation matrix and *then* calculate the Euler angles. Extra credit: show that the following surmise is correct. If a plane, hkl , is chosen in the lower hemisphere, $l < 0$, show that the Euler angles are *incorrect*.

Crystal Orientation: Axis-angle Pair

- Axis-angle pair is defined such that the crystal frame and the sample frame is overlapped by a single rotation, θ , along a common axis $[u \ v \ w]$.
- Commonly written as $(\hat{r}, \theta)$ or (n, ω)
- Active rotation
- The rotation can be converted to a matrix (*passive* rotation)
- Common in misorientation representation
 - Difference of misorientation vs. rotation difference is the choice of reference axis
- Easy conversion into Rodrigues-Frank vectors



Rotation matrices from Axis-angle

For $(\hat{r}, \theta)$ or (n, ω)

$$g_{ij} = \delta_{ij} \cos \theta + r_i r_j (1 - \cos \theta) + \sum_{k=1,3} \varepsilon_{ijk} r_k \sin \theta$$
$$= \begin{pmatrix} \cos \theta + u^2(1 - \cos \theta) & uv(1 - \cos \theta) + w \sin \theta & uw(1 - \cos \theta) - v \sin \theta \\ uv(1 - \cos \theta) - w \sin \theta & \cos \theta + v^2(1 - \cos \theta) & vw(1 - \cos \theta) + u \sin \theta \\ uw(1 - \cos \theta) + v \sin \theta & vw(1 - \cos \theta) - u \sin \theta & \cos \theta + w^2(1 - \cos \theta) \end{pmatrix}$$

This form of the rotation matrix is a *passive* rotation, appropriate to axis transformations

Axis-Angle from Rotation matrices

Rotation axis, $\mathbf{n}$:

$$\mathbf{n} = \frac{(a_{23} - a_{32}), (a_{31} - a_{13}), (a_{12} - a_{21})}{\sqrt{(a_{23} - a_{32})^2 + (a_{31} - a_{13})^2 + (a_{12} - a_{21})^2}}$$

Note the order (very important) of the coefficients in each subtraction; again, if the matrix represents an *active rotation*, then the sign is inverted.

Rotation angle, θ :

$$a_{ii} = 3\cos\theta + (1 - \cos\theta)n_i^2 = 1 + 2\cos\theta$$

therefore,

$$\cos\theta = 0.5(\text{trace}(a) - 1).$$

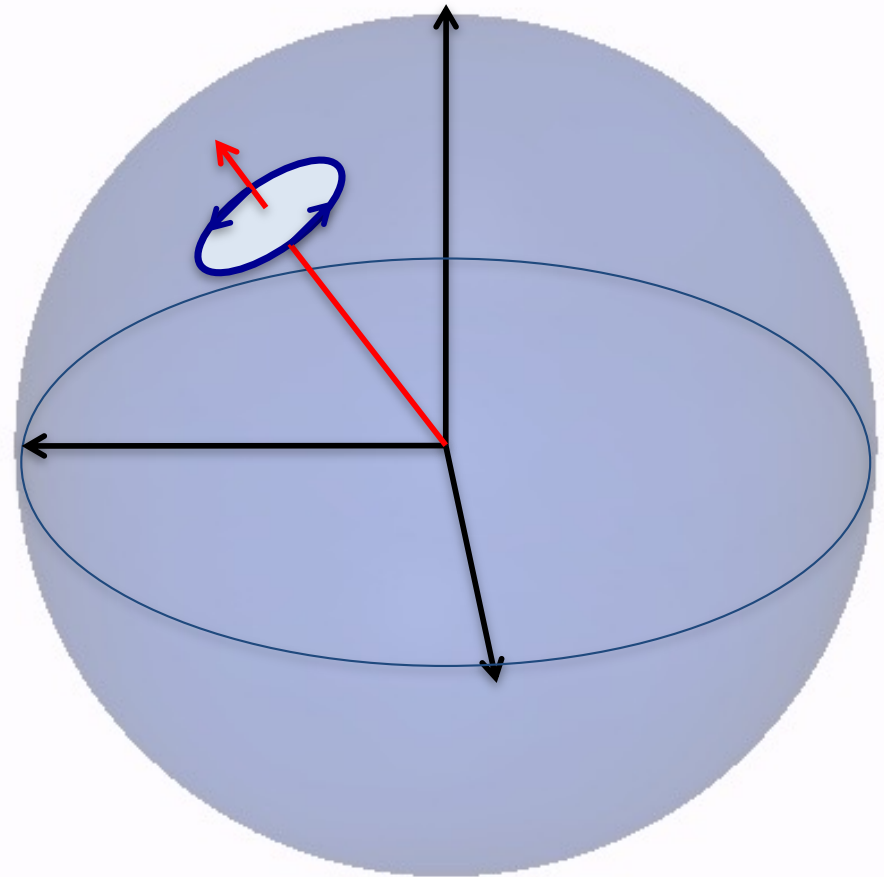
Crystal Orientation: Rodrigues-Frank Vectors

- Rodrigues vectors were popularized by Frank [“Orientation mapping.” *Metall. Trans.* **19A**: 403-408 (1988)], hence the term Rodrigues-Frank space
- Easily converted from axis-angle
- Most useful for representation of *misorientations*, also useful for orientations

The RF representation from axis angle $\mathcal{R}(r, \alpha)$ scales r by the tangent of $\alpha/2$

$$\rho = \hat{r} \tan(\alpha / 2)$$

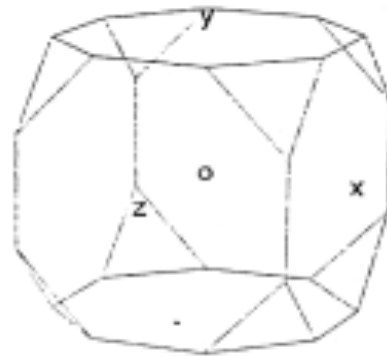
Note semi-angle



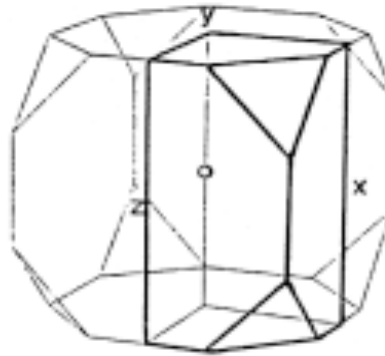
O. Rodrigues. “Des lois géométriques qui régissent les déplacements d'un système solide dans l'espace, et de la variation des coordonnées provenant de ces déplacements considérés indépendamment des causes qui peuvent les produire”, *Journal de mathématiques pures et appliquées*, **5**, 380-440 (1840).

Rodrigues-Frank Space

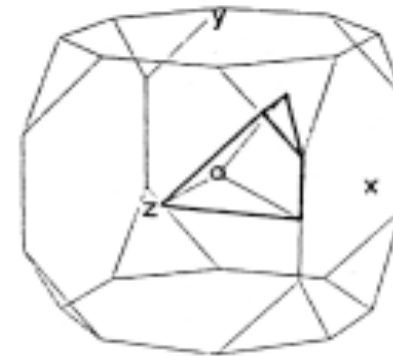
- Population of vectors
- Smallest R results from the smallest θ , and it lies closest to the origin of the RF space
- Lines in RF space represent rotation about fixed axis
- Further, when the RF space is divided into subvolumes, the misorientations that lie on the boundary of the subvolume are geometrically special, by having a low index axis of misorientation.
- As the Rodrigues vector is so closely linked to the rotation axis, which is meaningful for the crystallography of grain boundaries, the RF representation of misorientations is very common.



a)
Cubic crystal symmetry
no sample symmetry



b)
Cubic
orthorhombic



c)
Cubic
cubic

R-F Vector from Rotation matrices

- Simple formula, due to Morawiec:

$$\begin{pmatrix} \rho_1 \\ \rho_2 \\ \rho_3 \end{pmatrix} = \begin{bmatrix} (a_{23} - a_{32}) / [1 + \text{tr}(a)] \\ (a_{31} - a_{13}) / [1 + \text{tr}(a)] \\ (a_{12} - a_{21}) / [1 + \text{tr}(a)] \end{bmatrix}$$

Trace of a matrix:

$$\text{tr}(a) = a_{11} + a_{22} + a_{33}$$

R-F Vector from Bunge Euler angles and Bunge Euler from R-F vectors

- $\tan(\alpha/2) = \sqrt{\{ (1/[\cos(\Phi/2) \cos\{(\phi_1 + \phi_2)/2\}]^2 - 1 \}}$
- $\rho_1 = \tan(\Phi/2) [\cos\{(\phi_1 - \phi_2)/2\} / \cos\{(\phi_1 + \phi_2)/2\}]$
- $\rho_2 = \tan(\Phi/2) [\sin\{(\phi_1 - \phi_2)/2\} / [\cos\{(\phi_1 + \phi_2)/2\}]$
- $\rho_3 = \tan\{(\phi_1 + \phi_2)/2\}$

P. Neumann (1991). "Representation of orientations of symmetrical objects by Rodrigues vectors." Textures and Microstructures **14-18**: 53-58.

Conversion from Rodrigues to Bunge Euler angles:

$$\text{sum} = \text{atan}(R_3) ; \text{diff} = \text{atan} (R_2/R_1)$$

$$\phi_1 = \text{sum} + \text{diff}; \Phi = 2. * \text{atan}(R_2 * \cos(\text{sum}) / \sin(\text{diff})); \phi_2 = \text{sum} - \text{diff}$$

Rotation matrix from R-F vectors

- Due to Morawiec:

$$a_{ij} = \frac{1}{1 + \rho_l \rho_l} ([1 - \rho_l \rho_l] \delta_{ij} + 2\rho_i \rho_j + 2\epsilon_{ijk} \rho_k)$$

Example for the 12 entry:

$$\begin{aligned} a_{12} &= \frac{1}{1 + \rho_l \rho_l} ([1 - \rho_l \rho_l] \delta_{12} + 2\rho_1 \rho_2 + 2\rho_3) \\ &= \frac{2(\rho_1 \rho_2 + \rho_3)}{1 + \rho_l \rho_l} \end{aligned}$$

NB. Morawiec's Eq. on p.22 has a minus sign in front of the last term; this will give an active rotation matrix, rather than the passive rotation matrix seen here.

Crystal Orientation: Unit Quaternions

What is a quaternion?

A quaternion (1843 by Hamilton) is an ordered set of four real numbers $q_0, q_1, q_2,$ and q_3 .

Here, **i**, **j**, **k** are the familiar unit vectors that correspond to the x-, y-, and z-axes, resp.

$$\begin{aligned} q &= q_0 + \mathbf{i}q_1 + \mathbf{j}q_2 + \mathbf{k}q_3 \\ &= (q_0, q_1, q_2, q_3) \\ &= \underbrace{q_0}_{\text{Scalar part}} + \underbrace{\mathbf{q}}_{\text{Vector part}} \end{aligned}$$

- [1] Quaternion multiplication is non-commutative ($\mathbf{pq} \neq \mathbf{qp}$)
- [2] An extension to 2D complex numbers
- [3] Of the 4 components, one is a 'real' scalar number, and the other 3 form a vector in imaginary ijk space!

$$\mathbf{q} = q_0 + iq_1 + jq_2 + kq_3$$

$$i^2 = j^2 = k^2 = ijk = -1$$

$$i = jk = -kj$$

$$j = ki = -ik$$

$$k = ij = -ji$$

Quaternions as rotations

- A quaternion can represent a rotation by an angle θ around a unit axis $\mathbf{n} = (x \ y \ z)$:

$$\mathbf{q} = \begin{bmatrix} \cos \frac{\theta}{2} & x \sin \frac{\theta}{2} & y \sin \frac{\theta}{2} & z \sin \frac{\theta}{2} \end{bmatrix}$$

or

$$\mathbf{q} = \left\langle \cos \frac{\theta}{2}, n \sin \frac{\theta}{2} \right\rangle$$

Note the use of the semi-angle, just as in Rodrigues-Frank vectors

- Checking the magnitude of the quaternion, $q_0^2 + |\mathbf{q}|^2 = 1$

$$\begin{aligned} |\mathbf{q}| &= \sqrt{q_0^2 + q_1^2 + q_2^2 + q_3^2} \\ &= \sqrt{\cos^2 \frac{\theta}{2} + x^2 \sin^2 \frac{\theta}{2} + y^2 \sin^2 \frac{\theta}{2} + z^2 \sin^2 \frac{\theta}{2}} \\ &= \sqrt{\cos^2 \frac{\theta}{2} + \sin^2 \frac{\theta}{2} (x^2 + y^2 + z^2)} \\ &= \sqrt{\cos^2 \frac{\theta}{2} + \sin^2 \frac{\theta}{2} n^2} = \sqrt{\cos^2 \frac{\theta}{2} + \sin^2 \frac{\theta}{2}} \\ &= \sqrt{1} = 1 \end{aligned}$$

Unit!

A Quaternion & Its Negative

- It is the case that any given quaternion has a negative, $-q$, which represents the same rotation as q .
- This is easily understood in terms of the rotation axis n and angle, ω , and adding 2π to the angle, *i.e.*, going from (n, ω) to $(n, \omega + 2\pi)$.
- In practical terms, unit quaternions give us “double coverage” of proper rotations.
- In computation, one has to be careful about results from symmetry operations and conversions back to axis-angle and/or Rodrigues-Frank vectors.
- As discussed by Morawiec in his book, pp.38-39, there is a distinction in terms of direction of rotation that matters for angular momentum.

Unit Quaternion from Rotation Matrices

Formulae, due to Morawiec:

$$\cos \theta / 2 = 1/2 \sqrt{1 + \text{tr}(\Delta g)} \equiv q_4 = \pm \frac{\sqrt{1 + \text{tr}(\Delta g)}}{2}$$

Note: passive rotation/
axis transformation (axis
changes sign for for active
rotation)

$$q_i = \pm \frac{\varepsilon_{ijk} \Delta g_{jk}}{4 \sqrt{1 + \text{tr}(\Delta g)}}$$

$$\begin{pmatrix} q_1 \\ q_2 \\ q_3 \\ q_4 \end{pmatrix} = \begin{bmatrix} \pm [\Delta g(2,3) - \Delta g(3,2)] / 2 \sqrt{1 + \text{tr}(\Delta g)} \\ \pm [\Delta g(3,1) - \Delta g(1,3)] / 2 \sqrt{1 + \text{tr}(\Delta g)} \\ \pm [\Delta g(1,2) - \Delta g(2,1)] / 2 \sqrt{1 + \text{tr}(\Delta g)} \\ \pm \sqrt{1 + \text{tr}(\Delta g)} / 2 \end{bmatrix}$$

Note the coordination of choice of sign!

Rotation Matrices from Unit Quaternions

For $q = q_0 + \mathbf{i}q_1 + \mathbf{j}q_2 + \mathbf{k}q_3$

Orientation matrix:

$$g = \begin{bmatrix} 1 - 2q_2^2 - 2q_3^2 & 2q_1q_2 + 2q_0q_3 & 2q_1q_3 - 2q_0q_2 \\ 2q_1q_2 - 2q_0q_3 & 1 - 2q_1^2 - 2q_3^2 & 2q_2q_3 + 2q_0q_1 \\ 2q_1q_3 + 2q_0q_2 & 2q_2q_3 - 2q_0q_1 & 1 - 2q_1^2 - 2q_2^2 \end{bmatrix}$$

Quaternions are

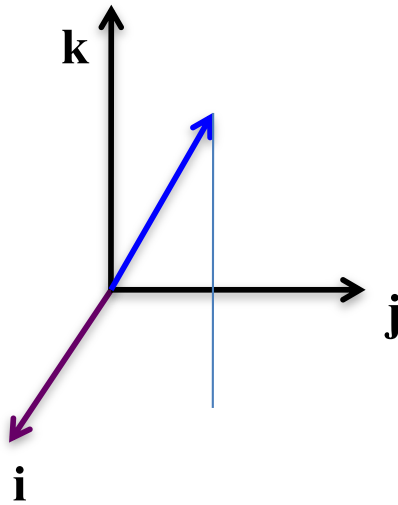
- Computationally efficient – multiplication requires fewer computations
- Axis-angle and R-F into quaternion conversion is simple

Rotation of a vector by a quaternion

$$\mathbf{w} = q^* \mathbf{v} q \quad \text{Passive rotation}$$

$$\mathbf{s} = q \mathbf{v} q^* \quad \text{Active rotation}$$

Consider rotating the vector $\mathbf{i}$ by an angle of $\alpha = 2\pi/3$ about the $\langle 111 \rangle$ direction.



For a *passive* rotation:

$$\begin{aligned} \mathbf{w} &= q^* \mathbf{i} q \\ &= \mathbf{k} \end{aligned}$$

$$\text{Rotation axis:} \quad \mathbf{r} = \left(1/\sqrt{3}, 1/\sqrt{3}, 1/\sqrt{3} \right)$$

$$\begin{aligned} q &= \cos(\alpha/2) + \mathbf{r} \sin(\alpha/2) \\ &= \frac{1}{2} + \left(\mathbf{i} \frac{1}{\sqrt{3}} + \mathbf{j} \frac{1}{\sqrt{3}} + \mathbf{k} \frac{1}{\sqrt{3}} \right) \frac{\sqrt{3}}{2} \end{aligned}$$

$$q_0 = \frac{1}{2} \quad \mathbf{q} = \frac{1}{2} \mathbf{i} + \frac{1}{2} \mathbf{j} + \frac{1}{2} \mathbf{k}$$

$$\mathbf{q} \cdot \mathbf{i} = \frac{1}{2} \quad \mathbf{q} \times \mathbf{i} = \frac{1}{2} \mathbf{j} - \frac{1}{2} \mathbf{k}$$

For an *active* rotation:

$$\begin{aligned} \mathbf{s} &= q \mathbf{i} q^* \\ &= \left(\frac{1}{4} - \frac{3}{4} \right) \mathbf{i} + 2 \left(\frac{1}{2} \right) \mathbf{q} + 2 \left(\frac{1}{2} \right) \left(\frac{1}{2} \mathbf{j} - \frac{1}{2} \mathbf{k} \right) \\ &= -\frac{1}{2} \mathbf{i} + \frac{1}{2} \mathbf{i} + \frac{1}{2} \mathbf{j} + \frac{1}{2} \mathbf{k} + \frac{1}{2} \mathbf{j} - \frac{1}{2} \mathbf{k} \\ &= \mathbf{j} \end{aligned}$$

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- Frank, F. (1988). "Orientation mapping," *Metallurgical Transactions* **19A**: 403-408.
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Properties of Quaternions

Magnitude of a quaternion:

$$|q|^2 = q^* q = q_0^2 + q_1^2 + q_2^2 + q_3^2$$

Conjugate of a quaternion:

$$\begin{aligned} q^* &= q_0 - \mathbf{q} \\ &= q_0 - \mathbf{i}q_1 - \mathbf{j}q_2 - \mathbf{k}q_3 \end{aligned}$$

Addition of quaternions:

$$p + q = (p_0 + q_0) + \mathbf{i}(p_1 + q_1) + \mathbf{j}(p_2 + q_2) + \mathbf{k}(p_3 + q_3)$$

Product of two arbitrary quaternions

$$\begin{aligned} pq &= p_0 q_0 - (p_1 q_1 + p_2 q_2 + p_3 q_3) \\ &\quad p_0 (\mathbf{i}q_1 + \mathbf{j}q_2 + \mathbf{k}q_3) + q_0 (\mathbf{i}p_1 + \mathbf{j}p_2 + \mathbf{k}p_3) \\ &\quad + \mathbf{i}(p_2 q_3 - p_3 q_2) + \mathbf{j}(p_3 q_1 - p_1 q_3) + \mathbf{k}(p_1 q_2 - p_2 q_1) \\ pq &= [p_0 q_0 - \mathbf{p} \cdot \mathbf{q}] + [p_0 \mathbf{q} + q_0 \mathbf{p} + \mathbf{p} \times \mathbf{q}] \\ &\quad \text{Scalar part} \qquad \text{Vector part} \end{aligned}$$

Using more compact notation:

again, note the + in front of the vector product

Cubic Crystal Symmetry Operators

Symmetry Operator		Rodrigues Vector	Unit Quaternion
2-fold on $\langle 100 \rangle$	L_{100}^2	$\infty(1,0,0)$ $\infty(0,1,0)$ $\infty(0,0,1)$	$\pm(1,0,0,0),$ $\pm(0,1,0,0)$ $\pm(0,0,1,0)$
4-fold on $\langle 100 \rangle$	L_{100}^4	$\pm(1,0,0)$ $\pm(0,1,0)$ $\pm(0,0,1)$	$\pm 1/\sqrt{2}(\pm 1,0,0,1),$ $\pm 1/\sqrt{2}(0,\pm 1,0,1)$ $\pm 1/\sqrt{2}(0,0,\pm 1,1)$
2-fold on $\langle 110 \rangle$	L_{110}^2	$\infty(1,\pm 1,0)$ $\infty(1,0,\pm 1)$ $\infty(0,1,\pm 1)$	$\pm 1/\sqrt{2}(\pm 1,1,0,0),$ $\pm 1/\sqrt{2}(0,1,\pm 1,0)$ $\pm 1/\sqrt{2}(\pm 1,0,1,0)$
3-fold on $\langle 111 \rangle$	L_{111}^3	$\pm(1,1,1)$ $\pm(1,-1,1)$ $\pm(1,1,-1)$ $\pm(-1,-1,1)$	$\pm 1/2(\pm 1,1,1,1),$ $\pm 1/2(1,-1,1,1),$ $\pm 1/2(1,1,-1,1),$ $\pm 1/2(-1,-1,1,1)$ $\pm 1/2(-1,1,-1,1),$ $\pm 1/2(1,-1,-1,1)$ $\pm 1/2(-1,-1,-1,1)$

The numerical values of these symmetry operators can be found at:

[http://pajarito.materials.cmu.edu/rollett/texture_subroutines: quat.cubic.symm](http://pajarito.materials.cmu.edu/rollett/texture_subroutines:quat.cubic.symm) etc²⁸

Combining Rotations as RF vectors

- Two Rodrigues vectors combine to form a third, ρ_C , as follows, where ρ_B follows after ρ_A . Note that this is *not* the parallelogram law for vectors!

$$\rho_C = (\rho_A, \rho_B) =$$

$$\{\rho_A + \rho_B - \rho_A \times \rho_B\} / \{1 - \rho_A \bullet \rho_B\}$$

addition

vector product

scalar product