Representation of Orientation
Lecture Objectives

- **Representation of Crystal Orientation**

  Stereography: *Miller indices, Matrices*

  3 Rotations: *Euler angles*

  Axis/Angle: *Rodriques Vector, Quaternion*

- **Texture component by a single point**


**Crystalline Nature of Materials**

- Many solid materials are composed of crystals joined together:
  - In metals and other materials, the individual grains may fit together closely to form the solid:
  - EBSD can determine the orientation of individual grains and characterize grain boundaries.
Crystalline Nature of Materials - Grains

- A grain is a region of discrete crystal orientation within a polycrystalline material.
- The grain boundary is the interface between individual grains.
- Grain boundaries have a significant influence on the properties of the material, dependant on the misorientation across boundaries.
A grain boundary is the interface between two neighbouring grains. Classified by the misorientation - the difference in orientation between two grains.

Grain boundaries are regions of comparative disorder, but, Special grain boundaries exist where a significant degree of order occurs

These are termed ‘CSL’ boundaries which have special properties
Crystalline Nature of Materials - CSLs

- Coincident Site Lattice boundaries (CSL's).
- A significant degree of order occurs at a CSL boundary, which leads to special properties.

Schematic representation of a \( \Sigma^3 \) boundary. Where the two grain lattices meet at the boundary, 1 in every 3 atoms is shared or coincident - shown in green.

Schematic representation of a \( \Sigma^5 \) boundary. 1 in every 5 atoms is shared or coincident.
Crystalline Nature of Materials - Properties

• Isotropic & Anisotropic Properties
  • If properties are equal in all directions, a material is termed 'Isotropic'.
  • If the properties tend to be greater or diminished in any direction, a material is termed 'Anisotropic'.
  • Many/most materials are anisotropic
  • Anisotropy results from preferred orientations or 'Texture'

In an isotropic polycrystalline material, grain orientations are random.
Crystalline Nature of Materials - Texture

• Texture may range from slight to highly developed
Orientation by Stereography
(Miller Index & Matrix)
Basic Crystallography - Bravais Lattices

• There are 14 Bravais Lattices:

• From these, 7 crystal systems are derived
Basic Crystallography - Crystal System

- Geometry of the unit cell
  → Repeated structure throughout the crystal.

### The Seven Crystal Systems

<table>
<thead>
<tr>
<th>Crystal system</th>
<th>Restrictions on the axial system</th>
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</thead>
<tbody>
<tr>
<td>Triclinic</td>
<td>( a \neq b \neq c ) ( \alpha \neq \beta \neq \gamma )</td>
</tr>
<tr>
<td>Monoclinic</td>
<td>( a \neq b \neq c ) ( \alpha = \beta = \gamma = 90 )</td>
</tr>
<tr>
<td>Orthorhombic</td>
<td>( a \neq b = c ) ( \alpha = \beta = \gamma = 90 )</td>
</tr>
<tr>
<td>Tetragonal</td>
<td>( a = b \neq c ) ( \alpha = \beta = \gamma = 90 )</td>
</tr>
<tr>
<td>Trigonal</td>
<td>( a = b = c ) ( \alpha = \beta = \gamma = 120 )</td>
</tr>
<tr>
<td>Hexagonal</td>
<td>( a = b = c ) ( \alpha = \beta = \gamma = 90 )</td>
</tr>
<tr>
<td>Cubic</td>
<td>( a = b = c ) ( \alpha = \beta = \gamma = 90 )</td>
</tr>
</tbody>
</table>

There are seven Crystal systems:

1. Cubic
2. Hexagonal
3. Trigonal
4. Tetragonal
5. Orthorhombic
6. Monoclinic
7. Triclinic

The lengths of the sides of the unit cell are shown below as \( a \), \( b \) and \( c \). The corresponding angles are shown as \( \alpha \), \( \beta \) and \( \gamma \).
Basic Crystallography – Crystallographic Direction

- A crystallographic direction describes the intersection of specific faces or lattice planes.
- Miller Indices can be used to describe directions.

For a cubic material the plane and the normal to the plane have the same indices.
For a cubic example, Miller indices can be derived to describe a plane.

Consider a cubic unit cell with sides $a, b, c$, with an origin as shown:

- Take reciprocal
- Miller Indices

$$\begin{align*}
a, b, c, & \quad 1, \infty, \infty, \\
1, \infty, \infty, & \quad 1, 1, \infty, \\
\infty, & \quad 1, 1, 1,
\end{align*}$$
Miller indices of a pole

Representation of Orientation
Stereographic Projection

- Uses the inclination of the normal to the crystallographic plane: the points are the intersection of each crystal direction with a (unit radius) sphere.

Fig. 2–25  \{100\} poles of a cubic crystal.
Projection from Sphere to Plane

- Projection of spherical information onto a flat surface
  - Equal area projection (Schmid projection)
  - Equiangular projection (Wulff projection, more common in crystallography)
Standard (001) Projection

Fig. 2–37 Standard (001) projection of a cubic crystal, after Barrett [1.7].

Representation of Orientation
**Stereographic, Equal Area Projections**

Stereographic (Wulff) Projection*:
\[ OP' = R \tan(\theta/2) \]

Equal Area (Schmid) Projection:
\[ OP' = R \sin(\theta/2) \]

* Many texts, e.g. Cullity, show the plane touching the sphere at N: this changes the magnification factor for the projection, but not its geometry.
Pole Figure Example

- If the Diffraction goniometer is set for \{100\} reflections, then all directions in the sample that are parallel to \langle100\rangle directions will exhibit diffraction.

→ The Sample shows a crystal oriented to put all 3 \langle100\rangle directions approximately equally spaced from the ND.
Miller Index of a Crystal Orientation

- 3 orthogonal directions as the reference frame. → a set of unit vectors called $e_1, e_2$ and $e_3$.

- In many cases we use the names Rolling Direction (RD) // $e_1$, Transverse Direction (TD) // $e_2$, and Normal Direction (ND) // $e_3$.

- We then identify a crystal (or plane normal) parallel to 3rd axis (ND) and a crystal direction parallel to the 1st axis (RD), written as (hkl)[uvw].
In this example the orientation of the crystal shown can be written as: \{100\}<110>
Basic Crystallography - Orientation Matrix

The orientation matrix describes the absolute orientation of the crystal with respect to the sample axes.
Euler Angles are a sequence of three angles which describe the rotation of a crystal with reference to crystal axes. The first is a rotation of $\phi_1$ about the crystal [001] (z), then $\Phi$ about the [100] (x), and finally $\phi_2$ about [001] (z).

- Euler Angles are the three rotations about the main crystal axes.
- Euler angles are one possible means of describing a crystal orientation.

Three rotations $\phi_1$, $\Phi$, $\phi_2$ about the Z, X, and Z axes are then quoted in degrees.
Basic Crystallography – Axis/Angle Misorientation

• Misorientation is the expression of the orientation of one crystal with respect to another crystal.

Representation of Orientation

Angle 60°

Misorientation = 60° [001]
Orientation by 3 Rotations
(Euler Angles : Mathematical Approach)
Euler Angle Definition (Bunge)

Representation of Orientation
Euler Angles, Animated

Crystal

Sample Axes

$e_3' = e_3 = \text{Z}_{\text{sample}} = \text{ND}$

$z_{\text{Crystal}} = e_3''''$

$e_2' = e_2 = \text{Y}_{\text{sample}} = \text{TD}$

$\varphi_2$

$e_3' = e_3''$

$e_1' = e_1''$

$\varphi_1$

$e_2'' = e_2''$

$e_1' = e_1''$

$\Phi$

$\Phi$

$[001]$

$[010]$

$[100]$

$3^{rd}$ position (final)

$2^{nd}$ position

$1^{st}$ position

Representation of Orientation
Euler Angles, Ship Analogy

Analogy: position and the heading of a boat with respect to the globe.

- **Latitude** ($\Theta$) and **longitude** ($\psi$)
  : Position of the boat on Earth
- third angle ($\phi$)
  : *heading of* boat relative to the line of longitude that connects the boat to the North Pole.
Meaning of Euler angles

- First two angles, $\phi_1$ and $\Phi$, the position of the [001] crystal direction relative to the specimen axes.
- Think of rotating the crystal about the ND (1st angle, $\phi_1$); then rotate the crystal out of the plane (about the [100] axis, $\Phi$);
- 3rd angle ($\phi_2$) tells Rotation of the crystal about [001].
Euler Angle Definitions

Bunge and Canova are inverse to one another
Kocks and Roe differ by sign of third angle
Bunge rotates about x’, Kocks about y’ (2nd angle)
## Conversions

<table>
<thead>
<tr>
<th>Convention</th>
<th>1&lt;sup&gt;st&lt;/sup&gt;</th>
<th>2&lt;sup&gt;nd&lt;/sup&gt;</th>
<th>3&lt;sup&gt;rd&lt;/sup&gt;</th>
<th>2&lt;sup&gt;nd&lt;/sup&gt; angle about t axis:</th>
</tr>
</thead>
<tbody>
<tr>
<td>Kocks (symmetric)</td>
<td>Ψ</td>
<td>Θ</td>
<td>φ</td>
<td>y</td>
</tr>
<tr>
<td>Bunge</td>
<td>ϕ&lt;sub&gt;1&lt;/sub&gt;−π/2</td>
<td>Φ</td>
<td>π/2−ϕ&lt;sub&gt;2&lt;/sub&gt;</td>
<td>x</td>
</tr>
<tr>
<td>Matthies</td>
<td>α</td>
<td>β</td>
<td>π−γ</td>
<td>y</td>
</tr>
<tr>
<td>Roe</td>
<td>Ψ</td>
<td>Θ</td>
<td>π−Φ</td>
<td>y</td>
</tr>
</tbody>
</table>
Miller indices to vectors

- Need the direction cosines for all 3 crystal axes.
- A direction cosine is the cosine of the angle between a vector and a given direction or axis.
- Sets of direction cosines can be used to construct a transformation matrix from the vectors.
Rotation of axes in the plane: $x, y = \text{old axes}; x', y' = \text{new axes}$

$$v' = \begin{pmatrix} \cos \theta & \sin \theta \\ -\sin \theta & \cos \theta \end{pmatrix} v$$

N.B. Passive Rotation/ Transformation of Axes
Definition of an Axis Transformation:

\[ \mathbf{e} = \text{old axes}; \quad \mathbf{e}' = \text{new axes} \]

Sample to Crystal (primed)

\[ a_{ij} = \mathbf{e}'_i \cdot \mathbf{e}'_j \]

\[
\begin{pmatrix}
  a_{11} & a_{12} & a_{13} \\
  a_{21} & a_{22} & a_{23} \\
  a_{31} & a_{32} & a_{33}
\end{pmatrix}
\]
Sample to Crystal (primed)

Miller index notation of texture component specifies direction cosines of xtal directions \( \parallel \) to sample axes.

\[
t = \text{hkl} \times \text{uvw}
\]
Form matrix from Miller Indices

\[ \hat{n} = \frac{(h, k, l)}{\sqrt{h^2 + k^2 + l^2}} \]
\[ \hat{b} = \frac{(u, v, w)}{\sqrt{u^2 + v^2 + w^2}} \]

\[ \hat{t} = \frac{\hat{n} \times \hat{b}}{|\hat{n} \times \hat{b}|} \]

Sample

\[ a_{ij} = \text{Crystal} \begin{pmatrix} b_1 & t_1 & n_1 \\ b_2 & t_2 & n_2 \\ b_3 & t_3 & n_3 \end{pmatrix} \]
**Bunge Euler angles to Matrix**

**Rotation 1** ($\phi_1$): rotate axes (anticlockwise) about the (sample) 3 [ND] axis; $Z_1$.

**Rotation 2** ($\Phi$): rotate axes (anticlockwise) about the (rotated) 1 axis [100] axis; $X$.

**Rotation 3** ($\phi_2$): rotate axes (anticlockwise) about the (crystal) 3 [001] axis; $Z_2$. 

**Representation of Orientation**
Bunge Euler angles to Matrix

\[ Z_1 = \begin{pmatrix} \cos \phi_1 & \sin \phi_1 & 0 \\ -\sin \phi_1 & \cos \phi_1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad X = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos \Phi & \sin \Phi \\ 0 & -\sin \Phi & \cos \Phi \end{pmatrix}, \]

\[ Z_2 = \begin{pmatrix} \cos \phi_2 & \sin \phi_2 & 0 \\ -\sin \phi_2 & \cos \phi_2 & 0 \\ 0 & 0 & 1 \end{pmatrix} \]

\[ A = Z_2 X Z_1 \]
Matrix with Bunge Angles

\[ A = Z_2 X Z_1 = \]

\[
\begin{bmatrix}
\cos \varphi_1 \cos \varphi_2 & \sin \varphi_1 \cos \varphi_2 \\
-\sin \varphi_1 \sin \varphi_2 \cos \Phi & +\cos \varphi_1 \sin \varphi_2 \cos \Phi \\
-\cos \varphi_1 \sin \varphi_2 & -\sin \varphi_1 \sin \varphi_2 \\
-\sin \varphi_1 \cos \varphi_2 \cos \Phi & +\cos \varphi_1 \cos \varphi_2 \cos \Phi \\
\sin \varphi_1 \sin \Phi & -\cos \varphi_1 \sin \Phi \\
\end{bmatrix}
\]

(hkl)

\[
\begin{bmatrix}
\sin \varphi_2 \sin \Phi \\
\cos \varphi_2 \sin \Phi \\
\cos \Phi \\
\end{bmatrix}
\]
Matrix, Miller Indices

- The general Rotation Matrix, $a$, can be represented as in the following:

\[
\begin{bmatrix}
    a_{11} & a_{12} & a_{13} \\
    a_{21} & a_{22} & a_{23} \\
    a_{31} & a_{32} & a_{33}
\end{bmatrix}
\]

- Where the Rows are the direction cosines for [100], [010], and [001] in the *sample coordinate system* (pole figure).
Matrix, Miller Indices

- The columns represent components of three other unit vectors:

\[
[uvw] \equiv RD
\]

\[
\begin{bmatrix}
  a_{11} & a_{12} & a_{13} \\
  a_{21} & a_{22} & a_{23} \\
  a_{31} & a_{32} & a_{33}
\end{bmatrix}
\]

\[
TD
\]

\[
ND \equiv (hkl)
\]

- Where the Columns are the direction cosines (i.e. hkl or uvw) for the RD, TD and Normal directions in the crystal coordinate system.
Compare Matrices

\[
\begin{bmatrix}
  b_1 & t_1 & n_1 \\
  b_2 & t_2 & n_2 \\
  b_3 & t_3 & n_3 \\
\end{bmatrix}
\text{Sample}
\]

\[
\begin{bmatrix}
  \cos \varphi_1 \cos \varphi_2 & \sin \varphi_1 \cos \varphi_2 \\
  -\sin \varphi_1 \sin \varphi_2 \cos \Phi & +\cos \varphi_1 \sin \varphi_2 \cos \Phi \\
  -\cos \varphi_1 \sin \varphi_2 & -\sin \varphi_1 \sin \varphi_2 \\
  -\sin \varphi_1 \cos \varphi_2 \cos \Phi & +\cos \varphi_1 \cos \varphi_2 \cos \Phi \\
  \sin \varphi_1 \sin \Phi & -\cos \varphi_1 \sin \Phi \\
\end{bmatrix}
\text{Crystal}
\]

\[
\begin{bmatrix}
  \sin \varphi_2 \sin \Phi \\
  \cos \varphi_2 \sin \Phi \\
  \cos \Phi \\
\end{bmatrix}
\text{(hkl)}
\]
Miller indices from Euler angle matrix

\[ h = n \sin \Phi \sin \varphi_2 \]
\[ k = n \sin \Phi \cos \varphi_2 \]
\[ l = n \cos \Phi \]
\[ u = n'(\cos \varphi_1 \cos \varphi_2 - \sin \varphi_1 \sin \varphi_2 \cos \Phi) \]
\[ v = n'(-\cos \varphi_1 \sin \varphi_2 - \sin \varphi_1 \cos \varphi_2 \cos \Phi) \]
\[ w = n' \sin \Phi \sin \varphi_1 \]

\( n, n' \) = factors to make integers
Euler angles from Miller indices

Inversion of the previous relations:

\[
\begin{align*}
\cos \Phi &= \frac{l}{\sqrt{h^2 + k^2 + l^2}} \\
\cos \varphi_2 &= \frac{k}{\sqrt{h^2 + k^2}} \\
\sin \varphi_1 &= \frac{w}{\sqrt{u^2 + v^2 + w^2}} \cdot \frac{\sqrt{h^2 + k^2 + l^2}}{\sqrt{h^2 + k^2}}
\end{align*}
\]

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.
Euler angles from Orientation Matrix

Notes:
The range of \( \cos^{-1} \) is 0-\( \pi \), which is sufficient for \( \Phi \) from this, \( \sin(\Phi) \) can be obtained.

The range of \( \tan^{-1} \) is 0-2\( \pi \), (must use the ATAN2 function) which is required for calculating \( \phi_1 \) and \( \phi_2 \).

\[
\Phi = \cos^{-1}(a_{33})
\]

\[
\varphi_2 = \tan^{-1}\left(\frac{a_{13}/\sin \Phi}{a_{23}/\sin \Phi}\right)
\]

\[
\varphi_1 = \tan^{-1}\left(\frac{a_{31}/\sin \Phi}{a_{32}/\sin \Phi}\right)
\]

if \( a_{33} \approx 1 \), \( \Phi = 0 \), \( \varphi_1 = \frac{\tan^{-1}(a_{12}/a_{11})}{2} \), and \( \varphi_2 = -\varphi_1 \)
Complete orientations in the Pole Figure

Note the loss of information in a diffraction experiment if each set of poles from a single component cannot be related to one another.
Complete Orientations in Inverse Pole Figure

Note the loss of information in a diffraction experiment if each set of poles from a single component cannot be related to one another. The same as Pole figure Experiment
Other Euler angle definitions

• Very **Confusing Aspect of Texture Analysis** is that there are multiple definitions of the Euler angles.
• Definitions according to *Bunge, Roe and Kocks* are in common use.
• Roe definition is Exactly Classical definition by Euler
• Components have *different values of Euler angles* depending on which definition is used.
• The *Bunge* definition is the most common.
• The differences between the definitions are based on differences in the sense of rotation, and the choice of rotation axis for the second angle.
Orientation by 3 Rotations
(Euler Angles : Texture Components)
Cube Component = \{001\}\langle100\rangle
Cube Texture (100)[001]:cube-on-face

- Observed in recrystallization of fcc metals
- The 001 orientations are parallel to the three ND, RD, and TD directions.
**Sharp Texture (Recrystallization)**

- Look at the (001) pole figures for this type of texture: maxima correspond to \{100\} poles in the standard stereographic projection.
Euler angles of Cube component

- The Euler angles for this component are simple, but not so simple!
- The crystal axes align exactly with the specimen axes, therefore all three angles are exactly zero: 
  \((\phi_1, \Phi, \phi_2) = (0^\circ, 0^\circ, 0^\circ)\).
- Due to the effects of crystal symmetry: aligning [100]//TD, [010]//-RD, [001]//ND. 
  \(\rightarrow\) evidently still the cube orientation 
  \(\rightarrow\) Euler angles are \((\phi_1, \Phi, \phi_2) = (90^\circ, 0^\circ, 0^\circ)\)!
\{011\}<001> : the Goss Component

- Goss Texture: Recrystallization texture for FCC materials such as Brass, ...
- \( (011) \) plane is oriented towards the ND and the [001] inside the \( (011) \) plane is along the RD.
\{011\}<001>: cube-on-edge

- In the 011 pole figure, one of the poles is oriented parallel to the ND (center of the pole figure) but the other ones will be at 60° or 90° angles but tilted 45° from the RD!
**Euler angles of Goss component**

- The Euler angles for this component are simple, and yet other variants exist, just as for the cube component.
- Only one rotation of 45° is needed to rotate the crystal from the reference position (i.e. the cube component); this happens to be accomplished with the 2nd Euler angle.
- \((\phi_1, \Phi, \phi_2) = (0^\circ, 45^\circ, 0^\circ)\).
  Other variants will be shown when symmetry is discussed.
Brass component

- Brass Texture: a rolling texture component for materials such as Brass, Silver, and Stainless steel.

(110)[112]
Brass component

- 30° Rotation of the Goss texture about the ND
Brass component: Euler angles

- The brass component is convenient because we can think about performing two successive rotations:
  - 1st about the ND, 2nd about the new position of the [100] axis.
  - 1st rotation is 35° about the ND; 2nd rotation is 45° about the [100].
  - \((\phi_1, \Phi, \phi_2) = (35°, 45°, 0°)\).
<table>
<thead>
<tr>
<th>Name</th>
<th>Indices</th>
<th>Bunge ((\varphi_1,\Phi,\varphi_2)) RD= 1</th>
<th>Kocks ((\psi,\Theta,\phi)) RD= 1</th>
<th>Bunge ((\varphi_1,\Phi,\varphi_2)) RD= 2</th>
<th>Kocks ((\psi,\Theta,\phi)) RD= 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>copper/1st var.</td>
<td>{112}〈111〉</td>
<td>40, 65, 26</td>
<td>50, 65, 26</td>
<td>50, 65, 64</td>
<td>39, 66, 63</td>
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<tr>
<td>copper/2nd var.</td>
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<td>S3*</td>
<td>{123}〈634〉</td>
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<tr>
<td>S/1st var.</td>
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<td>S/3rd var.</td>
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<td>64, 37, 63</td>
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<td>55, 45, 0</td>
<td>35, 45, 0</td>
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<td>55, 90, 45</td>
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<tr>
<td>brass/3rd var.</td>
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<td>55, 45, 90</td>
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<td>Taylor</td>
<td>{4 \ 4 \ 1}〈11 11 8〉</td>
<td>42, 71, 20</td>
<td>48, 71, 20</td>
<td>48, 71, 70</td>
<td>42, 71, 70</td>
</tr>
<tr>
<td>Taylor/2nd var.</td>
<td>{4 \ 4 \ 1}〈11 11 8〉</td>
<td>90, 27, 45</td>
<td>0, 27, 45</td>
<td>0, 27, 45</td>
<td>90, 27, 45</td>
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<td>Goss/1st var.</td>
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<td>0, 45, 0</td>
<td>90, 45, 0</td>
<td>90, 45, 0</td>
<td>0, 45, 0</td>
</tr>
<tr>
<td>Goss/2nd var.</td>
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<td>0, 45, 90</td>
</tr>
</tbody>
</table>
Summary

• Conversion between different forms of description of texture components described.

• Physical picture of the meaning of Euler angles as rotations of a crystal given.

• Miller indices are descriptive, but matrices are useful for computation, and Euler angles are useful for mapping out textures (to be discussed).
Orientation by Axis/Angle
(Rodrigues Vectors, Quaternions)
Objectives

• Introduction of Rodrigues* vector as a representation of rotations, orientations and misorientations (grain boundary types).

• Introduction of quaternion and its relationship to other representations

*French mathematician active in the early part of the 19th C.
Rodrigues vector

• Rodrigues vectors were popularized by Frank [Frank, F. (1988). “Orientation mapping.” Metallurgical Transactions 19A: 403-408.], hence the term Rodrigues-Frank space for the set of vectors.

• Most useful for representation of misorientations, i.e. grain boundary character; also useful for orientations (texture components).

• Fibers based on a fixed axis are always straight lines in RF space (unlike Euler space).
**Rodrigues vector**

- Axis-Angle representation:
  \[
  \mathbf{r} = \frac{\mathbf{OQ}}{|\mathbf{OQ}|} \quad \text{Rotation axis}
  \]
  \[
  \rho = r \tan\left(\frac{\alpha}{2}\right) \quad \text{Rotation Angle about Axis: } \alpha
  \]

The rotation angle is \( \alpha \), and the magnitude of the vector is scaled by the tangent of the semi-angle.

**BEWARE:** Rodrigues vectors do NOT obey the parallelogram rule (because rotations are NOT commutative!)

Representation of Orientation
Orientation, Misorientation

- **Orientation**: \( g \)
- **Misorientation**: \( \Delta g \)
- Given two orientations (grains) \( g_A \) and \( g_B \)
- Misorientation between A and B Orientation

\[ \Delta g = g_B g_A^{-1} \]
Conversions: Matrix $\rightarrow$ RF vector

- Conversion from rotation (misorientation) matrix: $\Delta g = g_B g_A^{-1}$

\[
\begin{pmatrix}
\rho_1 \\
\rho_2 \\
\rho_3
\end{pmatrix} = \begin{bmatrix}
\tan \frac{\theta}{2} \left[ \Delta g(2,3) - \Delta g(3,2) \right] / \text{norm} \\
\tan \frac{\theta}{2} \left[ \Delta g(1,3) - \Delta g(3,1) \right] / \text{norm} \\
\tan \frac{\theta}{2} \left[ \Delta g(1,2) - \Delta g(2,1) \right] / \text{norm}
\end{bmatrix}
\]

\[
\text{norm} = \sqrt{[\Delta g(2,3) - \Delta g(3,2)]^2 + [\Delta g(1,3) - \Delta g(3,1)]^2 + [\Delta g(1,2) - \Delta g(2,1)]^2}
\]

\[
\cos \frac{\theta}{2} = \sqrt{\frac{1}{2} (\cos \theta + 1)} = \frac{1}{2} \sqrt{1 + \text{tr}(\Delta g)}
\]
Conversion from Bunge Euler Angles:

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

“Representation of orientations of symmetrical objects by Rodrigues vectors.”
Combining Rotations as RF vectors

- Two Rodrigues vectors combine to form a third, $\rho_C$, as follows, where $\rho_B$ follows after $\rho_A$. Note: NOT parallelogram law for vectors!

$$\rho_C = (\rho_A, \rho_B) = \frac{\rho_A + \rho_B - \rho_A \times \rho_B}{1 - \rho_A \cdot \rho_B}$$

vector product  scalar product
Combining Rotations as RF vectors: component form

\[
\begin{aligned}
(\rho_1^C, \rho_2^C, \rho_3^C) &= \left( \frac{\rho_1^A + \rho_1^B - \left[ \rho_2^A \rho_3^B - \rho_3^A \rho_2^B \right]}{1 - \left( \rho_1^A \rho_1^B + \rho_2^A \rho_2^B + \rho_3^A \rho_3^B \right)} \right) \\
&\quad \left[ \rho_2^A + \rho_2^B - \left[ \rho_3^A \rho_1^B - \rho_1^A \rho_3^B \right] \right) \\
&\quad \left[ \rho_3^A + \rho_3^B - \left[ \rho_1^A \rho_2^B - \rho_2^A \rho_1^B \right] \right) \\
\end{aligned}
\]
Quaternions

- A close cousin to the Rodrigues vector
- A four component vector in relation to the axis-angle representation as follows
  - $[uvw]$ : Unit vector of rotation axis
  - $\theta$ : Rotation angle.
- $q = q(q_1,q_2,q_3,q_4)$
  - $= q(u \sin \theta/2, v \sin \theta/2, w \sin \theta/2, \cos \theta/2)$
Why Use Quaternions?

• Quaternions offer a efficient way on combining rotations, because of the small number of floating point operations required to compute the product of two rotations.

• The quaternion has a unit norm 
\[ \sqrt{q_1^2 + q_2^2 + q_3^2 + q_4^2} = 1 \] → Always Finite Value
→ No Computational Overflow & Underflow
Computation: combining rotations

- **Quaternions**
  - 16 multiplies and 12 additions
  - with no divisions or transcendental functions.
- **Matrix**
  - 27 multiplies and 18 additions.
- **Rodrigues vector**
  - 10 multiplies and 9 additions.
- The product of two rotations
  - the least work with Rodrigues vectors
Conversions: matrix → quaternion

\[
\begin{align*}
\begin{pmatrix} q_1 \\ q_2 \\ q_3 \\ q_4 \end{pmatrix} &= \\
&= \begin{bmatrix} 
\sin \frac{\theta}{2} \left[ \Delta g(2,3) - \Delta g(3,2) \right] / \text{norm} \\
\sin \frac{\theta}{2} \left[ \Delta g(1,3) - \Delta g(3,1) \right] / \text{norm} \\
\sin \frac{\theta}{2} \left[ \Delta g(1,2) - \Delta g(2,1) \right] / \text{norm} \\
\cos \frac{\theta}{2} 
\end{bmatrix} \\
\text{norm} &= \sqrt{\left[ \Delta g(2,3) - \Delta g(3,2) \right]^2 + \left[ \Delta g(1,3) - \Delta g(3,1) \right]^2 + \left[ \Delta g(1,2) - \Delta g(2,1) \right]^2} \\
\cos \frac{\theta}{2} &= \frac{1}{2} \sqrt{1 + \text{tr}(g)} \quad \sin \frac{\theta}{2} = \frac{1}{2} \sqrt{3 - \text{tr}(g)}
\end{align*}
\]
Conversions: quaternion → matrix

- The conversion of a quaternion to a rotation matrix is given by:
- \( e_{ijk} \) is the permutation tensor, \( \delta_{ij} \) the Kronecker delta

\[
g_{ij} = (q_4^2 - q_1^2 - q_2^2 - q_3^2) \delta_{ij} \\
+ 2q_i q_j + 2q_4 \sum_{k=1,3} e_{ijk} q_k
\]
Bunge angles → Quaternion

- \([q_1, q_2, q_3, q_4] = \)

  \[
  \begin{bmatrix}
  \sin \Phi/2 \cos\left\{ (\phi_1 - \phi_2)/2 \right\}, \\
  \sin \Phi/2 \sin\left\{ (\phi_1 - \phi_2)/2 \right\}, \\
  \cos \Phi/2 \sin\left\{ \phi_1 + \phi_2 \right\}/2, \\
  \cos \Phi/2 \cos\left\{ (\phi_1 + \phi_2)/2 \right\} 
  \end{bmatrix}
  \]

Note the occurrence of sums and differences of the 1\textsuperscript{st} and 3\textsuperscript{rd} Euler angles!
Combining quaternions

- The algebraic form for combination of quaternions is as follows, where $q_B$ follows $q_A$:

$$q_C = q_A q_B$$

$$q_{C1} = q_{A1}q_{B4} + q_{A4}q_{B1} - q_{A2}q_{B3} + q_{A3}q_{B2}$$

$$q_{C2} = q_{A2}q_{B4} + q_{A4}q_{B2} - q_{A3}q_{B1} + q_{A1}q_{B3}$$

$$q_{C3} = q_{A3}q_{B4} + q_{A4}q_{B3} - q_{A1}q_{B2} + q_{A2}q_{B1}$$

$$q_{C4} = q_{A4}q_{B4} - q_{A1}q_{B1} - q_{A2}q_{B2} - q_{A3}q_{B3}$$
Positive vs Negative Rotations

considering a rotation of \( \theta \) about an arbitrary axis, \( r \). If one rotates \textit{backwards} by the complementary angle, \( \theta - 2\pi \) (also about \( r \)), in terms of quaternions, however, \textbf{the representation is different}!
**Positive vs Negative Rotations**

Rotation $\theta$ about an axis, $\mathbf{r}$

\[
\mathbf{q}(\mathbf{r}, \theta) = \mathbf{q}(u \sin \theta/2, v \sin \theta/2, w \sin \theta/2, \cos \theta/2)
\]

Rotation $\theta - 2\pi$ about an axis, $\mathbf{r}$

\[
\mathbf{q}(\mathbf{r}, \theta - 2\pi) = \mathbf{q}(u \sin(\theta - 2\pi)/2, v \sin(\theta - 2\pi)/2, w \sin(\theta - 2\pi)/2, \cos(\theta - 2\pi)/2)
\]

\[
= \mathbf{q}(-u \sin \theta/2, -v \sin \theta/2, -w \sin \theta/2, -\cos \theta/2)
\]

\[
= -\mathbf{q}(\mathbf{r}, \theta)
\]

- The quaternion representing the negative rotation is the negative of the original (positive) rotation. The positive and negative quaternions are equivalent or physically indistinguishable, $\mathbf{q} \equiv -\mathbf{q}$. 

**Representation of Orientation**
**Negative of a Quaternion**

- The negative (inverse) of a quaternion is given by negating the fourth component, \( q^{-1} = \pm (q_1, q_2, q_3, -q_4) \); this relationship describes the *switching symmetry* at grain boundaries.

\[
I = q_A q_B
\]

\[
I = (0,0,0,1) \quad q_A = q_B^{-1}
\]
Summary

• Rodrigues vectors :
  → Rotations with a 3-component vector.
• Quaternions form a complete algebra.
  → In unit length quaternions, they are very useful for describing rotations.
  → Calculation of misorientations in cubic systems is particularly efficient.
**Matrix with Roe angles**

$$a(\psi, \theta, \phi) = [uvw] (hkl)$$

\[
\begin{pmatrix}
-\sin \psi \sin \phi & \cos \psi \sin \phi & -\cos \phi \sin \theta \\
+\cos \psi \cos \phi \cos \theta & +\sin \psi \cos \phi \cos \theta & \sin \phi \sin \theta \\
-\sin \psi \cos \phi & \cos \psi \cos \phi & \sin \phi \sin \theta \\
-\cos \psi \sin \phi \cos \theta & -\sin \psi \sin \phi \cos \theta & \cos \theta
\end{pmatrix}
\]
Roe angles $\rightarrow$ quaternion

\[ [q_1, q_2, q_3, q_4] = \]
\[
\begin{align*}
-\frac{\sin \Theta}{2} \sin\frac{(\Psi - \Phi)}{2}, \\
\sin \Theta/2 \cos\frac{(\Psi - \Phi)}{2}, \\
\cos \Theta/2 \sin\frac{(\Psi + \Phi)}{2}, \\
\cos \Theta/2 \cos\frac{(\Psi + \Phi)}{2}
\end{align*}
\]
Conversion from Roe Euler Angles:

- \( \tan(\theta/2) = \sqrt{(1/[\cos(\Theta/2) \cos((\Psi + \Phi)/2)]^2 - 1} \)
- \( \rho_1 = -\tan(\Theta/2) \sin((\Psi - \Phi)/2)/[\cos((\Psi + \Phi)/2)] \)
- \( \rho_2 = \tan(\Theta/2) \cos((\Psi - \Phi)/2)/[\cos((\Psi + \Phi)/2)] \)
- \( \rho_3 = \tan((\Psi + \Phi)/2) \)

See, for example, Altmann’s book on Quaternions, where \( \Psi = \alpha, \Theta = \beta, \Phi = \gamma \). These formulae can be converted to those on the previous page for Bunge angles by substituting:
\( \Psi = \phi_1 - \pi/2, \Phi = \phi_1 + \pi/2. \)
Matrix with Kocks Angles

\[
a(\Psi, \Theta, \phi) = \begin{bmatrix}
-\sin \Psi \sin \phi \\
-\cos \Psi \cos \phi \cos \Theta \\
\sin \Psi \cos \phi \\
-\cos \Psi \sin \phi \cos \Theta \\
\cos \Psi \sin \Theta
\end{bmatrix}
\begin{bmatrix}
-\sin \Psi \cos \phi \cos \Theta \\
-\cos \Psi \cos \phi \\
-\sin \Psi \sin \phi \cos \Theta \\
-\sin \Psi \sin \Theta \\
\sin \Psi \sin \Theta \\
\cos \Theta
\end{bmatrix}
\]

(hkl)

Note: obtain transpose by exchanging \( \phi \) and \( \Psi \).