Polycrystalline Diffraction - A Primer for the 2018 APS NX School

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Overview

This document is a compilation of notes from *MAE 7110 Micromechanical Modeling and Diffraction Experiments for Crystalline Solids* a course in Mechanical and Aerospace Engineering at Cornell University taught by CHESS beamline scientist, Darren Pagan, and Matt Miller. Darren Pagan created a series of 8 lectures based on this course that are posted on youtube (https://www.youtube.com/channel/UCRXIeRvDOlfS88EXDGH2yeQ/playlists). The focus of MAE 7110 is the use of a new class of synchrotron-based High Energy X-ray Diffraction (HEXD) experiments that have evolved over the past decade at CHESS, APS Sector 1, the ESRF and other light sources around the world (cf. [1]). These experiments take advantage of the penetration power of high energy x-rays, *in situ* loading / heating environments and high speed area detectors to literally "watch" individual crystals within a polycrystalline aggregate deform during loading. Mechanics and micromechanics are the emphasis and these data are especially useful when used together with multiscale material modeling formulations [2]. The notes are a mixture of x-ray science, materials engineering and solid mechanics designed to train graduate students in the use of HEXD data to understand the deformation-induced distributions of stress and orientation in a deforming aggregate. In particular, the use of the HEXD data in conjunction with material behavior models is emphasized. The course is biased towards engineers who need to develop an understanding of reciprocal space and diffraction and are mainly interested in the grain scale elastic-plastic deformation behavior of metallic polycrystals. After a primer on indicial notation, vectors and tensors, a general description of crystallography and diffraction is presented. The details of modeling a diffraction experiment from a continuum mechanics perspective is presented followed by a description of crystal-scale mechanics from the perspective of diffraction. Some references are included. The notes are not necessarily a "how to" do these experiments, but between the notes and the youtube videos, an untrained user can get enough training to show up at a beamline with an idea about what to do. There are no doubt inconsistencies and mistakes throughout - please let us know (mpm4@cornell.edu) when you find one/many. Good luck!

Contents

1 Some Elements of Solid Mechanics

1.1 Direct Notation

- In direct notation, vectors are written in bold font while tensors are written in bold font and sometimes underlined: $\boldsymbol{v}$, $\underline{\boldsymbol{\sigma}}$, $\underline{\boldsymbol{a}}$
- Basis vectors (unit) : $\mathbf{\hat{e}_1}$, $\mathbf{\hat{e}_2}$, $\mathbf{\hat{e}_3}$. Sometimes the hats aren't there.

  Vector:

$$\mathbf{v} = v_1\mathbf{\hat{e}_1} + v_2\mathbf{\hat{e}_2} + v_3\mathbf{\hat{e}_3} \tag{1}$$

  2nd order tensor:

$$\begin{aligned} \phi = \phi_{11}\mathbf{\hat{e}_1\hat{e}_1} + \phi_{12}\mathbf{\hat{e}_1\hat{e}_2} + \phi_{13}\mathbf{\hat{e}_1\hat{e}_3} + \\ \phi_{21}\mathbf{\hat{e}_2\hat{e}_1} + \phi_{22}\mathbf{\hat{e}_2\hat{e}_2} + \phi_{23}\mathbf{\hat{e}_2\hat{e}_3} \\ +\phi_{31}\mathbf{\hat{e}_3\hat{e}_1} + \phi_{32}\mathbf{\hat{e}_3\hat{e}_2} + \phi_{33}\mathbf{\hat{e}_3\hat{e}_3} \end{aligned} \tag{2}$$

  or

$$\begin{aligned} \phi = \phi_{11}\mathbf{\hat{e}_1} \otimes \mathbf{\hat{e}_1} + \phi_{12}\mathbf{\hat{e}_1} \otimes \mathbf{\hat{e}_2} + \phi_{13}\mathbf{\hat{e}_1} \otimes \mathbf{\hat{e}_3} + \\ \phi_{21}\mathbf{\hat{e}_2} \otimes \mathbf{\hat{e}_1} + \phi_{22}\mathbf{\hat{e}_2} \otimes \mathbf{\hat{e}_2} + \phi_{23}\mathbf{\hat{e}_2} \otimes \mathbf{\hat{e}_3} \\ +\phi_{31}\mathbf{\hat{e}_3} \otimes \mathbf{\hat{e}_1} + \phi_{32}\mathbf{\hat{e}_3} \otimes \mathbf{\hat{e}_2} + \phi_{33}\mathbf{\hat{e}_3} \otimes \mathbf{\hat{e}_3} \end{aligned} \tag{3}$$

1.2 Indicial Notation

- We often choose to only write the components of a vector: i.e. v_1, v_2, v_3, i.e. v_i where i can take on values from 1-3. We do the same thing with second or fourth order tensors, ϕ_{ij} and C_{ijkl}, respectively.

Rules / definitions:

- An index can appear once or twice within a term but never more than twice.
- Repeated indices are called dummy and implies summation over the range, i.e. $\phi_{ii} = \phi_{11} + \phi_{22} + \phi_{33}$
- Unrepeated indices indicate the order of the term, 0=scalar, 1=vector (first order tensor) 2 = second order tensor...

Vector operations:

- $u_i = x_i - X_i$ is actually 3 equations: $i = 1, i = 2, i = 3$.
- $u_i = x_i - X_A$ has no meaning
- Dot product: $\mathbf{u} \cdot \mathbf{v} = (u_i\mathbf{\hat{e}_i}) \cdot (v_j\mathbf{\hat{e}_j}) = u_i v_j(\mathbf{\hat{e}_i} \cdot \mathbf{\hat{e}_j})$, For regular Cartesian Coordiantes (RCC) $(\mathbf{\hat{e}_i} \cdot \mathbf{\hat{e}_j}) = 1$ for $i = j$ or 0 for $i \neq j$ (kronecker delta, δ_{ij}), so $u_i v_j(\mathbf{\hat{e}_i} \cdot \mathbf{\hat{e}_j}) = u_i v_j \delta_{ij} = u_i v_i = u_1 v_1 + u_2 v_2 + u_3 v_3$
- Outer product $\mathbf{uv} = \mathbf{u} \otimes \mathbf{v} = (u_i v_j)(\mathbf{\hat{e}_i\hat{e}_j}) = (u_i v_j)(\mathbf{\hat{e}_i} \otimes \mathbf{\hat{e}_j})$
- Cross product: $\mathbf{u} \times \mathbf{v} = (u_i\mathbf{\hat{e}_i}) \times (v_j\mathbf{\hat{e}_j}) = u_i v_j(\mathbf{\hat{e}_i} \times \mathbf{\hat{e}_j})$ (for RCC, i.e. $(\mathbf{\hat{e}_1} \times \mathbf{\hat{e}_1}) = 0$ and $(\mathbf{\hat{e}_1} \times \mathbf{\hat{e}_2}) = \mathbf{\hat{e}_3}$...

- The permutation (Levi Civita) tensor handles things like cross product:

$$\begin{aligned}\epsilon_{ijk} &= 1 \text{ for } i,j,k = 1,2,3 \text{ or permutation}\\ &= -1 \text{ for } i,j,k = 2,1,3 \text{ or permutation}\\ &= 0 \text{ for any repeated indices}\end{aligned}$$

- Now $(u_i\mathbf{\hat{e}_i}) \times (v_j\mathbf{\hat{e}_j}) = u_i v_j(\mathbf{\hat{e}_i} \times \mathbf{\hat{e}_j}) = \epsilon_{ijk}u_i v_j\mathbf{\hat{e}_k} = w_k\mathbf{\hat{e}_k}$ or leave off the basis vector for pure indicial notation: $\epsilon_{ijk}u_i v_j = w_k$

- Note: don't get ϵ_{ijk} confused with the strain tensor, ϵ_{ij} (3 indices instead of 2). Also e_{ijk} is sometimes used for the permutation symbol.

- Scalar Triple Product:

$$\begin{aligned}\mathbf{u}\cdot(\mathbf{v}\times\mathbf{w}) &= (u_i\mathbf{\hat{e}_i})\cdot(v_j\mathbf{\hat{e}_j}\times w_k\mathbf{\hat{e}_k})\\ &= (u_i\mathbf{\hat{e}_i})\cdot(\epsilon_{jkl}v_j w_k\mathbf{\hat{e}_l})\\ &= u_i\epsilon_{jkl}v_j w_k\delta_{il}\\ &= \epsilon_{jkl}v_j w_k u_l \qquad (4)\end{aligned}$$

- Vector Triple Product:

$$\begin{aligned}\mathbf{u}\times(\mathbf{v}\times\mathbf{w}) &= (u_i\mathbf{\hat{e}_i})\times(v_j\mathbf{\hat{e}_j}\times w_k\mathbf{\hat{e}_k})\\ &= (u_i\mathbf{\hat{e}_i})\times(\epsilon_{jkl}v_j w_k\mathbf{\hat{e}_l})\\ &= \epsilon_{ilm}u_i\epsilon_{jkl}v_j w_k\mathbf{\hat{e}_m} \qquad (5)\end{aligned}$$

- Differentiation:
  Use a comma to denote spatial differentiation, i.e. $\frac{\partial u_i}{\partial x_j} = u_{i,j}$ or $\frac{\partial \sigma_{ji}}{\partial x_j} = \sigma_{ji,j}$

Tensors and Matrices

- Dyad $\equiv \mathbf{ab}$ or $\mathbf{a}\otimes\mathbf{b} = (a_i b_j)(\mathbf{\hat{e}_i\hat{e}_j}) = (a_i b_j)(\mathbf{\hat{e}_i}\otimes\mathbf{\hat{e}_j})$

- A second order tensor ($\underline{\boldsymbol{\phi}}$) transforms one vector ($\mathbf{a}$) to another ($\mathbf{b}$): $\mathbf{b} = \underline{\boldsymbol{\phi}}\cdot\boldsymbol{a}$;

$$\boldsymbol{b} = b_i\boldsymbol{\hat{e}_i} = \phi_{ij}\boldsymbol{\hat{e}_i}\boldsymbol{\hat{e}_j}\cdot a_k\boldsymbol{\hat{e}_k} = \underline{\boldsymbol{\phi}}\cdot\boldsymbol{a} \qquad (6)$$

$$\boldsymbol{b} = b_i\boldsymbol{\hat{e}_i} = \phi_{ij}a_k\boldsymbol{\hat{e}_i}(\boldsymbol{\hat{e}_j}\cdot\boldsymbol{\hat{e}_k}) = \phi_{ij}a_k\boldsymbol{\hat{e}_i}\delta_{jk} = \phi_{ij}a_j\boldsymbol{\hat{e}_i} \qquad (7)$$

$$b_i = \phi_{ij}a_j \qquad (8)$$

- In this course we will use a matrix notation at times, in which matrices of numbers are listed as scripted letters: $\underline{\boldsymbol{A}} = A_{ij}$ or $\boldsymbol{a} = a_i$
- Dot product of two second order tensors is another second order tensor: $A_{ij}B_{jk} = C_{ik}$

- Scalar product of two second order tensors is a scalar: $A_{ij}B_{ij} = c$

1.3 Coordinate Transformations

- Building the transformation matrix that takes the components of a vector or second order tensor from one coordinate system or basis into another basically happens by considering components of a vector in each coordinate system using dot products with the basis vectors: the original or "old" basis, $\hat{\mathbf{e}}_\mathbf{i}$, to a new one, $\hat{\mathbf{e}}'_\mathbf{i}$. (For example crystal to sample or crystal to laboratory)

- A vector can be written in either $\mathbf{v} = v_i\hat{\mathbf{e}}_\mathbf{i} = v'_i\hat{\mathbf{e}}'_\mathbf{i}$. We will determine the value of a component of $\mathbf{v}$, v'_j by projecting $\mathbf{v}$ written using the old basis onto the new basis vector $\hat{\mathbf{e}}'_\mathbf{i}$ using the dot product:

$$v'_i\hat{\boldsymbol{e}}'_i = v_i\hat{\boldsymbol{e}}_i. \tag{9}$$

- Taking the dot product of both sides with $\hat{\boldsymbol{e}}^S_j$ (the 'new' coordinate system):

$$v'_i(\hat{\boldsymbol{e}}'_i \cdot \hat{\boldsymbol{e}}'_j) = v_i(\hat{\boldsymbol{e}}_i \cdot \hat{\boldsymbol{e}}'_j). \tag{10}$$

- We define the coordinate transformation a_{ij} ($\underline{\boldsymbol{a}}$) as:

$$\underline{\boldsymbol{a}} = a_{ij} = \hat{\boldsymbol{e}}'_i \cdot \hat{\boldsymbol{e}}_j \tag{11}$$

$$v'_i\delta_{ij} = v_i(a_{ji}). \tag{12}$$

$$v'_j = a_{ji}v_i. \tag{13}$$

- or in matrix form:

$$\boldsymbol{v'} = \begin{bmatrix} v'_1 \\ v'_2 \\ v'_3 \end{bmatrix} = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{23} & a_{33} \end{bmatrix} \begin{bmatrix} v_1 \\ v_2 \\ v_3 \end{bmatrix} = \underline{\boldsymbol{a}}\boldsymbol{v} \tag{14}$$

- *Note the ordering of basis vectors in equation 11. This gives

$$\hat{\boldsymbol{e}}'_{\boldsymbol{i}} = A_{ij}\hat{\boldsymbol{e}}_{\boldsymbol{j}} \tag{15}$$

- so for example:

$$\hat{\boldsymbol{e}}'_1 = (\hat{\boldsymbol{e}}'_1 \cdot \hat{\boldsymbol{e}}_1)\hat{\boldsymbol{e}}_1 + (\hat{\boldsymbol{e}}'_1 \cdot \hat{\boldsymbol{e}}_2)\hat{\boldsymbol{e}}_2 + (\hat{\boldsymbol{e}}'_1 \cdot \hat{\boldsymbol{e}}_3)\hat{\boldsymbol{e}}_3. \tag{16}$$

- Be really careful here about the connection between the indices of the dot product and the indices of the transformation matrix. For instance, we have defined it this way $a_{ij} = \hat{\mathbf{e}}'_\mathbf{i}\cdot\hat{\mathbf{e}}_\mathbf{j} = \hat{\mathbf{e}}_\mathbf{j}\cdot\hat{\mathbf{e}}'_\mathbf{i} = a_{\textbf{new old}}$. This is the definition used by most of the solid mechanics community but some (composites guys...) may use the opposite, $a_{\textbf{old new}}$. The transformation rules will just be reversed, nothing crazy needs to happen beyond that.

- For a second order tensor, think of building the tensor using the outer product of two vectors,

$$\underline{\mathbf{M}} = \mathbf{uv} = M_{ij}\hat{\mathbf{e}}_\mathbf{i}\hat{\mathbf{e}}_\mathbf{j} = M'_{ij}\hat{\mathbf{e}}'_\mathbf{i}\hat{\mathbf{e}}'_\mathbf{j} = u_iv_j\hat{\mathbf{e}}_\mathbf{i}\hat{\mathbf{e}}_\mathbf{j} = u'_iv'_j\hat{\mathbf{e}}'_\mathbf{i}\hat{\mathbf{e}}'_\mathbf{j} \tag{17}$$

- Now, take the version in the new coordinate system u'_i and v'_j and use the dot product to project onto the old system,

$$u'_i v'_j = u_k(\mathbf{\hat{e}_k} \cdot \mathbf{\hat{e}'_i}) v_l(\mathbf{\hat{e}_l} \cdot \mathbf{\hat{e}'_j}) = u_k A_{ik} v_l A_{jl} = M'_{ij} = M_{kl} A_{ik} A_{jl}$$

- Basically this defines how you would code this up: $\boldsymbol{M'} = \boldsymbol{aMa}^T$. You can think of applying the "vector" transformation to the basis vector associated with each index. So the transformation of a fourth order tensor is , $C'_{ijkl} = a_{I'm} a_{jn} a_{ko} a_{lp} C_{mnop}$.

1.4 Stress and Strain

The Cauchy stress, σ_{ij} is defined with the normal vector to a cutting plane, n_i and the traction vector, $t_i^{\mathbf{n}}$ as $t_i^{\mathbf{n}} = \sigma_{ji} n_j$. All transformation rules apply, $\sigma'_{ij} = a_{ik} a_{jl} \sigma_{kl}$. We determine the principal values of stress or any second order tensor using the characteristic equations derived from the concept of the traction vector aligning with the normal vector (no shear stress on principal planes), i.e. $\det([\sigma] - \lambda [I]) = 0$. The characteristic equation is then $\lambda^3 - I_1 \lambda^2 - I_2 \lambda - I_3 = 0$, where the λs are the principal values (eigenvalues) and each has its own principal direction (eigenvector). The stress invariants are defined as:

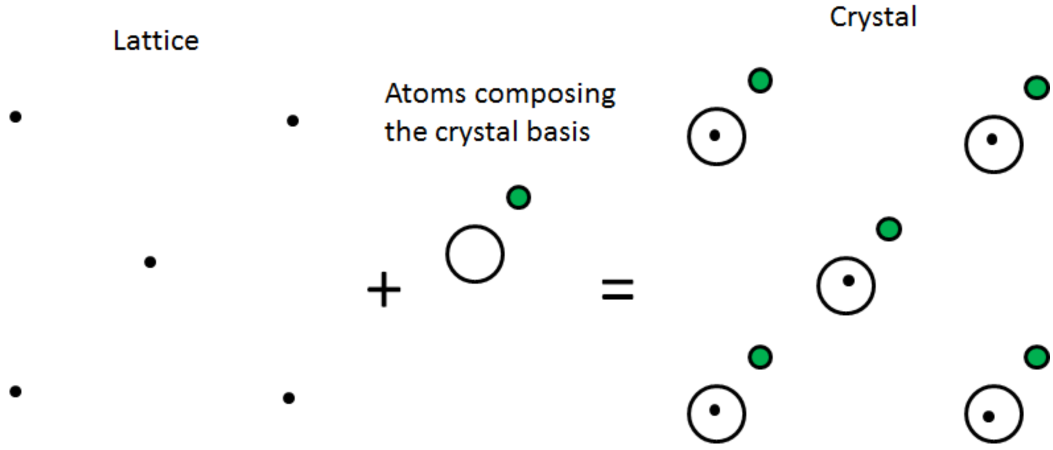
$$\begin{aligned} I_1 &= \sigma_{kk} \\ I_2 &= \frac{1}{2}\left(\sigma_{ii}\sigma_{jj} - \sigma_{ij}\sigma_{ji}\right) \\ I_3 &= \frac{1}{6}\left(2\sigma_{ij}\sigma_{jk}\sigma_{ki} - 3\sigma_{ij}\sigma_{ji}\sigma_{kk} + \sigma_{ii}\sigma_{jj}\sigma_{kk}\right) \end{aligned}$$

We will primarily use the infinitesimal strain tensor, defined as $\epsilon_{ij} = \frac{1}{2}(u_{i,j} + u_{j,i})$ where u_i is the displacement vector. In much of what we do, the strains are elastic. A general form of Hooke's law for anisotropic elasticity is presented later. However, plasticity is also considered (primarily at the slip system level). Hopefully this distinction will be clear. In the final chapter of this document, a more complete description of large strain deformation is presented.

2 Crystallography, Orientations and Symmetry

2.1 Basic Crystallography

- This focus here is on the study of the deformation of crystals, typically within a polycrystal.
- Crystals are solids with a *periodic* arrangement of atoms.
- The ability to study crystals using X-ray diffraction is a consequence of this periodicity, as we will discuss later.
- Crystallography is a very deep subject. However, this section will focus on providing the basics so that we can study changes to a crystal *with a known crystal structure* due to mechanical deformation using X-ray diffraction.
- Crystals are mathematically described by a *lattice* and a *crystal basis* (motif)
- Formally, the crystal is described by a *convolution* (which we will discuss later) of the lattice and the crystal basis. A convolution is sometimes described as a tiling or folding operation. The crystal basis is 'tiled' on to every lattice point, generating the complete crystal.



- Lattices:
  - A lattice is a set of periodically spaced points that are 'fixed' to the crystal.
  - The surroundings of each lattice point are identical. (To help visualize this, imagine we are viewing a lattice point in a crystal. We then close our eyes and the crystal is shifted so that a different lattice point is now in front of us. If we then open our eyes, we wouldn't be able to tell that the crystal had been moved.)
  - In three dimensions, a crystal unit cell is define by three lattice basis vectors. We will call these vectors $\boldsymbol{a_1}$, $\boldsymbol{a_2}$, and $\boldsymbol{a_3}$ (they will sometimes be referred to as direct lattice basis vectors).
  - Therefore, the position of the origin of each unit cell is given by:

$$\boldsymbol{x_{uvw}} = u\boldsymbol{a_1} + v\boldsymbol{a_2} + w\boldsymbol{a_3} \tag{18}$$

  - where u, v, and w are integers. The integers $[uvw]$ placed in brackets is shorthand for a crystallographic direction. The $< uvw >$in parentheses describes a set of symmetrically equivalent directions (we will discuss crystal symmetry later). Bars placed over the integers indicate negative signs.

    - For example, in a cubic lattice, [100] and [$\bar{1}$00] crystal directions are both part of the $< 100 >$ family of crystal directions.
- The region of the crystal enclosed by $\boldsymbol{a_1}$, $\boldsymbol{a_2}$, and $\boldsymbol{a_3}$ is called the *unit cell* of the crystal
- The volume V of the unit cell is:

$$V = \boldsymbol{a_1} \cdot (\boldsymbol{a_2} \times \boldsymbol{a_3}) \tag{19}$$

- The unit cell can also be described completely using the parameters a, b, c, α, β, and γ, where:

$$a = ||\boldsymbol{a_1}|| \tag{20a}$$
$$b = ||\boldsymbol{a_2}|| \tag{20b}$$
$$c = ||\boldsymbol{a_3}|| \tag{20c}$$
$$\alpha = \angle(\boldsymbol{a_2}, \boldsymbol{a_3}) \tag{20d}$$
$$\beta = \angle(\boldsymbol{a_1}, \boldsymbol{a_3}) \tag{20e}$$
$$\gamma = \angle(\boldsymbol{a_1}, \boldsymbol{a_2}) \tag{20f}$$

- A crystal coordinate system with basis ($\hat{\boldsymbol{e}}_i^C$) must also be associated with the lattice basis vectors. One of the most used conventions can be found in Busing and Levy, 1967. In this convention
    - $\boldsymbol{a_1}$ is parallel to $\hat{\boldsymbol{e}}_1^C$
    - $\boldsymbol{a_2}$ is in the plane defined by $\hat{\boldsymbol{e}}_1^C$ and $\hat{\boldsymbol{e}}_2^C$
    - $\boldsymbol{a_3}$ is arbitrary
- Symmetry restricts the possible lattice types to the 14 Bravais lattice types (listed in Cullity and Stock pg. 44)
- The choice of lattice basis vectors and unit cell origin is arbitrary (again as long as the periodicity of the lattice is maintained and the unit cell is space filling). However, by convention some unit cell choices are better than others:

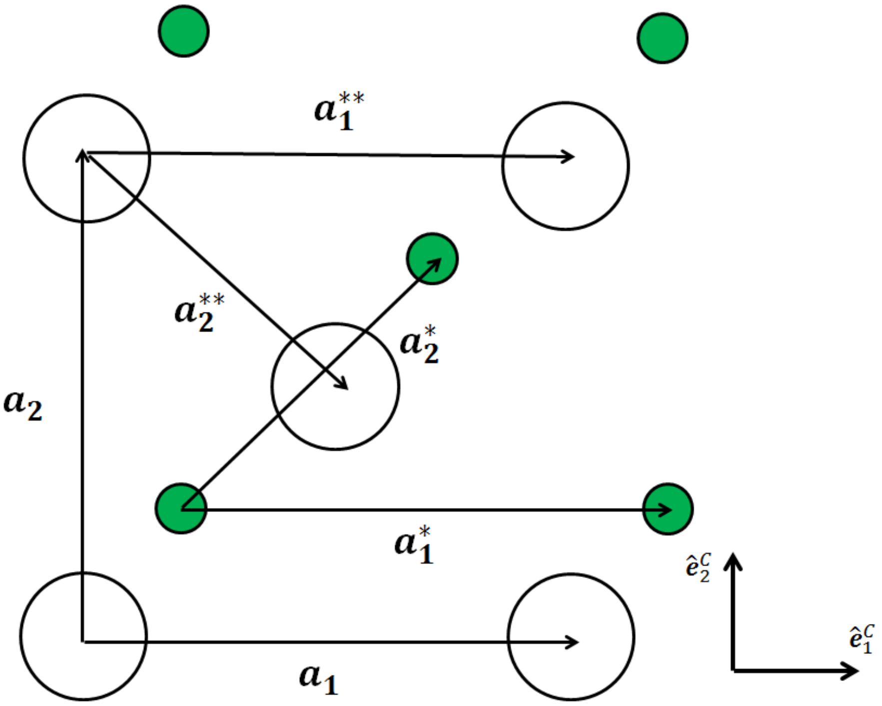
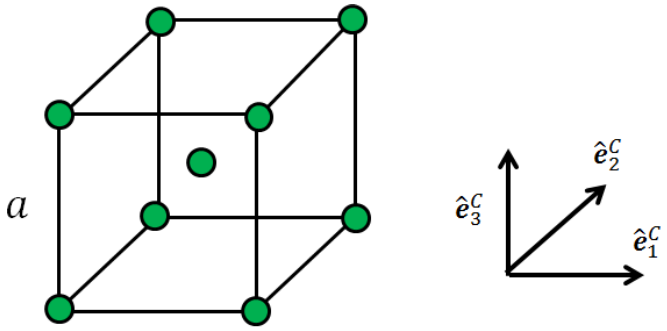


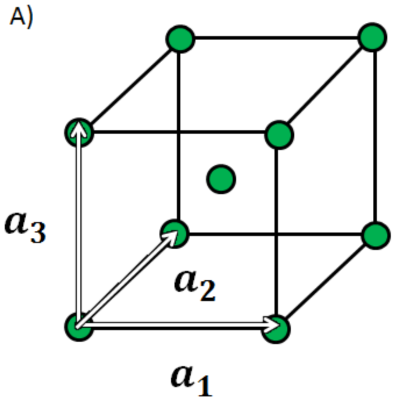
Figure 1: Different Lattice Basis Vectors Choices

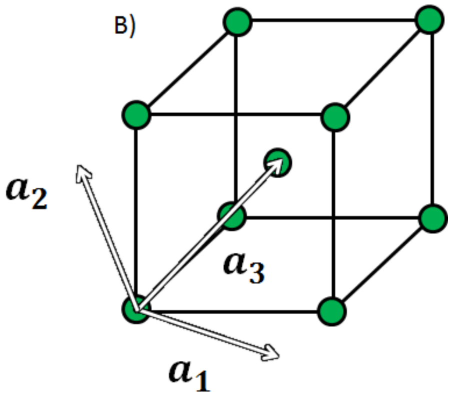
- ∗ A *primitive* unit cell is a unit cell which encloses the smallest possible volume and a single lattice point per unit cell.
- ∗ The origin of each unit cell is often chosen to be the center of an atom.
- ∗ Figure 1 shows examples of different choices of lattice basis vectors in 2-D. *Note that $\boldsymbol{a}_i^*$ and $\boldsymbol{a}_i^*{*}$ are primitive.

- Crystal Bases:
  - The crystal bases describe the positions of atoms (or more formally, the charge density or potential energy) within each unit cell. The atomic positions are often described with fractions of the lattice basis vectors.
  - *Note: The definition of the crystal basis changes with choice of lattice basis vectors, so take care that you know the definition of the lattice basis vectors when you find atomic positions in reference.

Example: Choosing a basis in a BCC crystal with one atom per lattice point.







A) Cubic Basis Vectors

If we pick the standard unit cell choice (cubic) with orthogonal basis vectors in the crystal coordinate system.

$$\boldsymbol{a}_1^C = a_0 \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}, \boldsymbol{a}_2^C = a_0 \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}, \boldsymbol{a}_3^C = a_0 \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}$$

With this choice, atom positions are:

$$\boldsymbol{z}_1 = 0\boldsymbol{a}_1 + 0\boldsymbol{a}_2 + 0\boldsymbol{a}_3$$

$$\boldsymbol{z}_2 = \tfrac{1}{2}\boldsymbol{a}_1 + \tfrac{1}{2}\boldsymbol{a}_2 + \tfrac{1}{2}\boldsymbol{a}_3$$

B) Basis Vectors Associated with a Primitive Unit Cell

$$\boldsymbol{a}_1^C = \frac{2a_0}{\sqrt{3}} \begin{bmatrix} \frac{1}{2} \\ \frac{1}{2} \\ -\frac{1}{2} \end{bmatrix}, \boldsymbol{a}_2^C = \frac{2a_0}{\sqrt{3}} \begin{bmatrix} -\frac{1}{2} \\ \frac{1}{2} \\ \frac{1}{2} \end{bmatrix}, \boldsymbol{a}_3^C = \frac{2a_0}{\sqrt{3}} \begin{bmatrix} \frac{1}{2} \\ \frac{1}{2} \\ \frac{1}{2} \end{bmatrix}$$

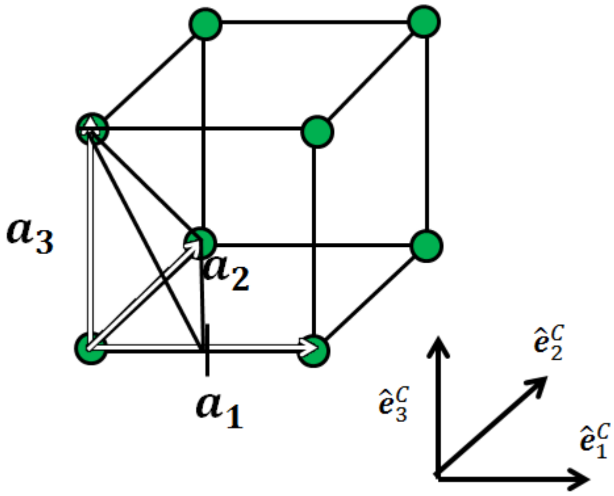
These lattice basis vectors are from the origin to three atoms (of 8 possible) nearest to the origin. With this choice, there is only one atom in the unit cell.

$$\boldsymbol{z}_1 = 0\boldsymbol{a}_1 + 0\boldsymbol{a}_2 + 0\boldsymbol{a}_3$$

- Lattice Planes:
  - A set of lattice planes are planes that are periodically spaced throughout the crystal. These planes are parallel as they are spaced throughout the crystal.

- The sets of lattice planes are described by how often they are periodically spaced (usually just called the lattice plane spacing) d and the orientation of the normal to the planes $\boldsymbol{n}$
- From measurements of the lattice plane spacing and orientation using X-ray diffraction, we can deduce the current state of the lattice.
- Sets of lattice planes are denoted by their Miller indices. The Miller indices of a lattice plane set (h,k, and l) are found by determining where the lattice planes intercept the 3 basis vectors of the unit cell. For example, if the Miller indices of a set of lattice planes are given by h,k, and l, the lattice planes will intercept the basis vectors at $\frac{1}{h}\boldsymbol{a_1}$, $\frac{1}{k}\boldsymbol{a_2}$, and $\frac{1}{l}\boldsymbol{a_3}$ respectively.
- A set of (hkl) surrounded by parentheses denotes a set of lattice planes, while $\{hkl\}$ denotes a family of symmetrically equivalent lattice planes. ((111) and $(1\bar{1}1)$ are both members of the $\{111\}$ family of lattice planes.
- The orientation of the lattice planes can be described by the vector normal to the lattice plane, $\boldsymbol{\hat{n}_{hkl}}$

Example: Finding the (211) lattice planes and their plane normal in a cubic crystal.



The (211) lattice planes intersect the basis vectors at $\frac{1}{2}\boldsymbol{a_1}$, $\boldsymbol{a_2}$, and $\boldsymbol{a_3}$. The vectors, ($\boldsymbol{v_1} = \boldsymbol{a_3} - \frac{1}{2}\boldsymbol{a_1}$) and ($\boldsymbol{v_2} = \boldsymbol{a_3} - \boldsymbol{a_2}$) both lie within the (211) plane. Therefore, their cross product must be normal to the (211) plane.

$$\boldsymbol{v_1} \times \boldsymbol{v_2} = (\boldsymbol{a_3} \times \boldsymbol{a_3}) - (\boldsymbol{a_3} \times \boldsymbol{a_2}) - \tfrac{1}{2}(\boldsymbol{a_1} \times \boldsymbol{a_3}) + \tfrac{1}{2}(\boldsymbol{a_1} \times \boldsymbol{a_2}) = \boldsymbol{a_1} + \tfrac{1}{2}\boldsymbol{a_2} + \tfrac{1}{2}\boldsymbol{a_3}$$

*Note that this direction is parallel to the [211] crystallographic direction. In cubic materials, the $[hkl]$ direction is perpendicular to the (hkl) lattice planes.

- The Reciprocal Lattice:
  - We will find that its often more convenient to describe diffraction from a crystal using the crystal's *reciprocal lattice.*
  - The reciprocal lattice is completely a construct, but we will be using it throughout the semester, so we should become comfortable.

- The basis vectors of the reciprocal lattice ($\boldsymbol{b_1}$, $\boldsymbol{b_2}$, and $\boldsymbol{b_3}$)

$$\boldsymbol{b_1} = \frac{2\pi}{V}(\boldsymbol{a_2} \times \boldsymbol{a_3}) \tag{21a}$$

$$\boldsymbol{b_2} = \frac{2\pi}{V}(\boldsymbol{a_3} \times \boldsymbol{a_1}) \tag{21b}$$

$$\boldsymbol{b_3} = \frac{2\pi}{V}(\boldsymbol{a_1} \times \boldsymbol{a_2}) \tag{21c}$$

- where V is the unit cell volume.
- *some alternative definitions use 1 instead of 2π, but by including the 2π will save ourselves lots of writing in derivations and calculations.
- The basis vectors given in Equation 21 satisfy the relationship:

$$\boldsymbol{a_i} \cdot \boldsymbol{b_j} = 2\pi\delta_{ij} \tag{22}$$

- Reciprocal lattice vectors $\boldsymbol{g}_{hkl}$ are linear combinations of the reciprocal lattice basis vectors.

$$\boldsymbol{g_{hkl}} = h\boldsymbol{b_1} + k\boldsymbol{b_2} + l\boldsymbol{b_3} \tag{23}$$

- These reciprocal lattice points have convenient relationships with the lattice planes that have the same Miller indices (hkl).
  - The spacing of the lattice planes (d_{hkl}) is given by:

$$d_{hkl} = \frac{2\pi}{||\boldsymbol{g_{hkl}}||} \tag{24}$$

  - Each reciprocal lattice point is parallel to the lattice plane normal of the associated lattice plane set:

$$\boldsymbol{\hat{n}_{hkl}} = \frac{\boldsymbol{g_{hkl}}}{||\boldsymbol{g_{hkl}}||} \tag{25}$$

- So through measurement of g_{hlk}, we can determine both the spacing and orientation of the associated lattice planes.

Example: Finding the spacing of the (331) lattice planes in a hexagonal crystal using the reciprocal lattice. The unit cell parameters are $a = b = 3\mathring{A}$, $c = 5\mathring{A}$, $\alpha = \beta = 90$, $\gamma = 120$.

$$\boldsymbol{a_1^C} = \begin{bmatrix} 3 \\ 0 \\ 0 \end{bmatrix} \mathring{A}, \boldsymbol{a_2^C} = \begin{bmatrix} -1.5 \\ 2.6 \\ 0 \end{bmatrix} \mathring{A}, \boldsymbol{a_3^C} = \begin{bmatrix} 0 \\ 0 \\ 5 \end{bmatrix} \mathring{A}$$

$$\boldsymbol{b_1^C} = \begin{bmatrix} 2.1 \\ 1.2 \\ 0 \end{bmatrix} \tfrac{1}{\mathring{A}}, \boldsymbol{b_2^C} = \begin{bmatrix} 0 \\ 2.4 \\ 0 \end{bmatrix} \tfrac{1}{\mathring{A}}, \boldsymbol{b_3^C} = \begin{bmatrix} 0 \\ 0 \\ 1.3 \end{bmatrix} \tfrac{1}{\mathring{A}}$$

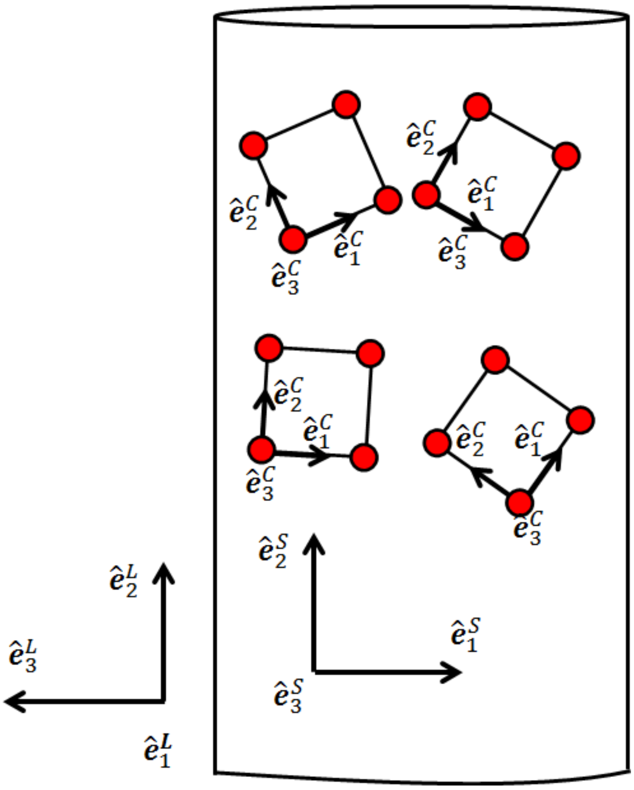
$$\boldsymbol{g}_{331}^C = \begin{bmatrix} \boldsymbol{b_1^C} \boldsymbol{b_2^C} \boldsymbol{b_3^C} \end{bmatrix} \begin{bmatrix} h \\ k \\ l \end{bmatrix} = \begin{bmatrix} 2.1 & 0 & 0 \\ 1.2 & 2.4 & 0 \\ 0 & 0 & 1.3 \end{bmatrix} \begin{bmatrix} 3 \\ 3 \\ 1 \end{bmatrix} \tfrac{1}{\mathring{A}} = \begin{bmatrix} 6.2 \\ 10.8 \\ 1.3 \end{bmatrix} \tfrac{1}{\mathring{A}}$$

$$d_{331} = \tfrac{2\pi}{||\boldsymbol{g_{hkl}}||} = 0.50\mathring{A}$$

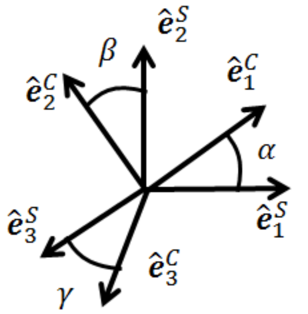
$$\hat{\boldsymbol{n}}^C_{331} = \begin{bmatrix} 0.50 \\ 0.86 \\ 0.11 \end{bmatrix}$$

2.2 Orientations

- In this course, we are often interested in determining *crystallographic orientation* of a volume (or many volumes) of crystal.
- The crystallographic orientation describes the positions of atomic lattice planes with respect to an external reference frame. (Randle and Engler)
- In our case we wish to describe the crystallographic orientation with respect to a sample or laboratory coordinate system.



- We need a way to describe crystallographic orientations, so first we will fix an orthanormal coordinate system to our crystal ($\hat{\boldsymbol{e}}_i^C$) and another to an external coordinate system($\hat{\boldsymbol{e}}_i^S$).
- The crystal orientation is defined by three independent piece of information. For example, the angles between basis vectors of our two coordinate systems uniquely define their relationship.



- We will define the crystal orientation with respect to the sample coordinate system ($\boldsymbol{R}^{S,C}$), (refer back to the review notes, if necessary)

$$\hat{\boldsymbol{e}}_i^S = R_{ij}^{S,C}\hat{\boldsymbol{e}}_j^C \tag{26}$$

- with this definition we find the transformation of a vector $\boldsymbol{v}$ from the crystal to sample coordinate systems as:

$$\boldsymbol{v}^S = v_i^S = R_{ij}^{S,C}v_j^C = \boldsymbol{R}^{S,C}\boldsymbol{v}^C \tag{27}$$

- A few general notes about coordinate transformations:
  - Successive coordinate transformations are generally not commutative:

$$\boldsymbol{R_2R_1} \neq \boldsymbol{R_1R_2} \tag{28}$$

  - The matrix product of a coordinate transformations with its transpose is identity:

$$\boldsymbol{RR}^T = \boldsymbol{I} \tag{29}$$

  since

$$\delta_{ij} = \hat{\boldsymbol{e}}_i' \cdot \hat{\boldsymbol{e}}_j' = R_{ik}\hat{\boldsymbol{e}}_{\boldsymbol{k}} \cdot R_{jl}\hat{\boldsymbol{e}}_{\boldsymbol{l}} = R_{ik}R_{jl}(\hat{\boldsymbol{e}}_k \cdot \hat{\boldsymbol{e}}_l') = R_{ik}R_{jk} \tag{30}$$

    * These 6 equations reduce the number of independent values of $\boldsymbol{R}$ from 9 to 3, so $\boldsymbol{R}$ only has 3 independent pieces of information as stated previously.
  - The transpose of a rotation is equal to its inverse:

$$\boldsymbol{RR}^T = \boldsymbol{I} = \boldsymbol{RR}^{-1} \tag{31}$$

$$\boldsymbol{R}^{-1} = \boldsymbol{R}^T \tag{32}$$

- Common Parameterizations of Orientations:
  - Rotation Matrices:
    * When a coordinate transformation is expressed as a matrix, it is referred to as a *Rotation Matrix*. We will use (and have been using) $\boldsymbol{R}$ to describe rotation matrices.
    * Coordinate transformations in which the two coordinate systems share a common basis vector have the forms:

    - $\hat{\boldsymbol{e}}_1' = \hat{\boldsymbol{e}}_1$

$$[\boldsymbol{R}] = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos(\phi) & \sin(\phi) \\ 0 & -\sin(\phi) & \cos(\phi) \end{bmatrix} \tag{33}$$

    - $\hat{\boldsymbol{e}}_2' = \hat{\boldsymbol{e}}_2$

$$[\boldsymbol{R}] = \begin{bmatrix} \cos(\phi) & 0 & -\sin(\phi) \\ 0 & 1 & 0 \\ \sin(\phi) & 0 & \cos(\phi) \end{bmatrix} \tag{34}$$

    - $\hat{\boldsymbol{e}}_3' = \hat{\boldsymbol{e}}_3$

$$[\boldsymbol{R}] = \begin{bmatrix} \cos(\phi) & \sin(\phi) & 0 \\ -\sin(\phi) & \cos(\phi) & 0 \\ 0 & 0 & 1 \end{bmatrix} \tag{35}$$

    - *Note that these matrices corresponds to the new coordinate system (primed) being rotated clockwise with respect to the old coordinate system (unprimed). The sign of the sine term will switch if the rotation is counterclockwise. Rotations around $\hat{\boldsymbol{e}}_2$ and $\hat{\boldsymbol{e}}_3$ are similar, except with permuted values.

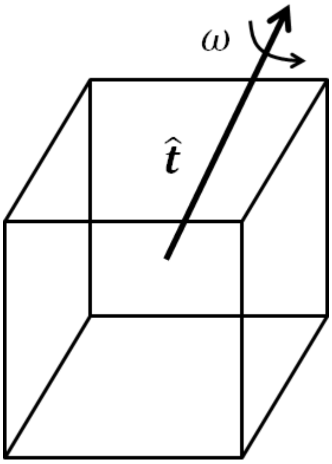
- Euler Angles:
    - Any coordinate transformation can be described as a sequence of coordinate transformations which share a common coordinate system basis vector systems axes (for example ($\hat{\boldsymbol{e}}_1 = \hat{\boldsymbol{e}}_1'$, $\hat{\boldsymbol{e}}_2' = \hat{\boldsymbol{e}}_2''$, $\hat{\boldsymbol{e}}_3'' = \hat{\boldsymbol{e}}_3'''$).
    - The angles about which the coordinate system axes are rotated are referred to as *Euler Angles.*
    - A common convention are Bunge angles which share the common axes $\hat{\boldsymbol{e}}_3 = \hat{\boldsymbol{e}}_3'$, $\hat{\boldsymbol{e}}_1' = \hat{\boldsymbol{e}}_1''$, $\hat{\boldsymbol{e}}_3'' = \hat{\boldsymbol{e}}_3'''$ is given by:

$$\boldsymbol{R} = \boldsymbol{R}_{\boldsymbol{\varphi_2}} \boldsymbol{R}_{\boldsymbol{\Phi}} \boldsymbol{R}_{\boldsymbol{\varphi_1}} =$$

$$\begin{bmatrix} \cos(\varphi_2) & \sin(\varphi_2) & 0 \\ -\sin(\varphi_2) & \cos(\varphi_2) & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos(\Phi) & \sin(\Phi) \\ 0 & -\sin(\Phi) & \cos(\Phi) \end{bmatrix} \begin{bmatrix} \cos(\varphi_1) & \sin(\varphi_1) & 0 \\ -\sin(\varphi_1) & \cos(\varphi_1) & 0 \\ 0 & 0 & 1 \end{bmatrix} \tag{36}$$

    - The evaluated rotation matrix can be found in Randle and Engler pg 27.

- Angle Axis Parameterizations:
    - All rotations can be described by a single axis ($\hat{\boldsymbol{t}}$) and an angle of rotation (ω) about that axis.



- There exists a family of angle axis parameterizations of angle axis combinations of the form:

$$\boldsymbol{r} = f(\omega)\boldsymbol{t} \tag{37}$$

- We will frequently be using Rodrigues vectors, which have the form:

$$\boldsymbol{r} = \tan(\omega/2)\boldsymbol{t} \tag{38}$$

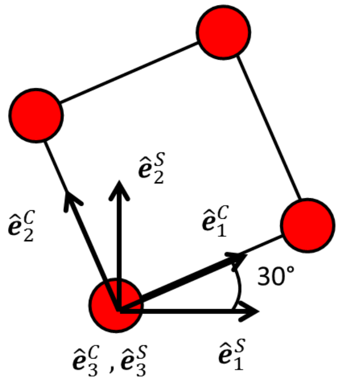
- The use of Rodrigues vectors has the benefits that fibers of orientations are straight lines in orientation space and reducing the space of all possible orientations because of crystal symmetry is straight forward.
- The components of a coordinate transformation $\boldsymbol{R}$ can be found from an angle and axis using the formula:

$$R_{ij} = \cos(\omega)\delta_{ij} - \sin(\omega)\epsilon_{ijk}\hat{t}_k + (1-\cos(\omega))\hat{t}_i\hat{t}_j \tag{39}$$

.

Example: Transforming the components of a vector in a crystal coordinate system to a sample coordinate system.

We want to find what the components of the $\boldsymbol{v}^C = \frac{1}{\sqrt{2}}[110]$ direction in the crystal coordinate system are in the the sample coordinate system.



$$\hat{\boldsymbol{e}}_1^S = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}, \hat{\boldsymbol{e}}_2^S = \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}, \hat{\boldsymbol{e}}_3^S = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}$$

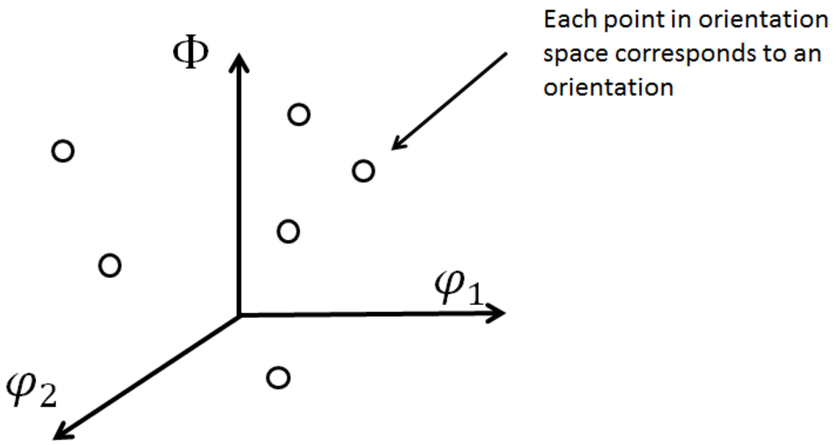
$$\hat{\boldsymbol{e}}_1^C = \begin{bmatrix} \cos(30) \\ \sin(30) \\ 0 \end{bmatrix}, \hat{\boldsymbol{e}}_2^C = \begin{bmatrix} -\sin(30) \\ \cos(30) \\ 0 \end{bmatrix}, \hat{\boldsymbol{e}}_3^C = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}$$

$$\boldsymbol{R}^{S,C} = \begin{bmatrix} \cos(30) & -\sin(30) & 0 \\ \sin(30 & \cos(30) & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

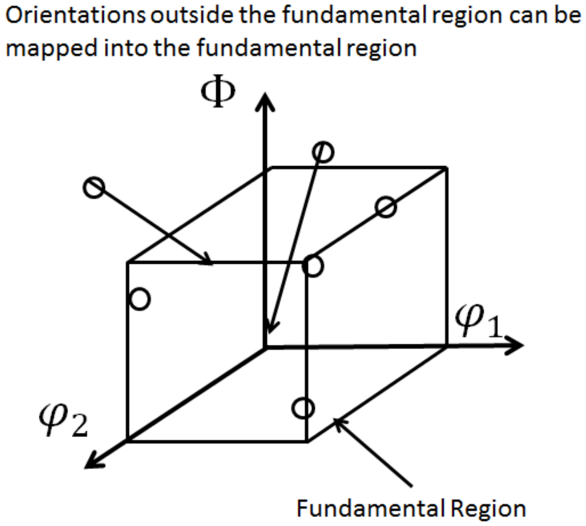
Finding the crystal direction in the sample coordinate system:

$$\boldsymbol{v}^S = \boldsymbol{R}^{S,C}\boldsymbol{v}^C = \frac{1}{\sqrt{2}} \begin{bmatrix} \cos(30) & -\sin(30) & 0 \\ \sin(30 & \cos(30) & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 \\ 1 \\ 0 \end{bmatrix} = \frac{1}{\sqrt{2}} \begin{bmatrix} \cos(30) - \sin(30) \\ \sin(30) + \cos(30) \\ 0 \end{bmatrix}$$

- Orientation Spaces and Orientation Distribution Function:
  - Since all orientations contain 3 pieces of information, all possible orientations with respect to an external coordinate system can be represented in a 3-D space called *orientation space*.



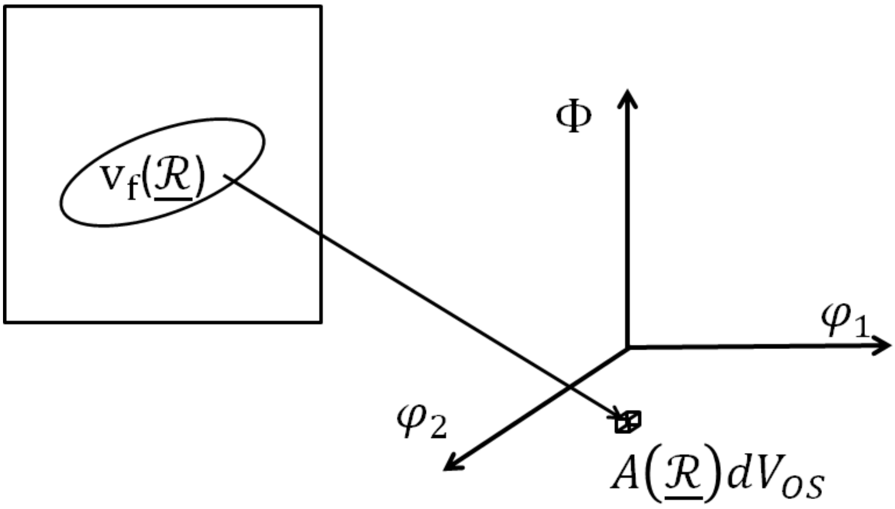
  - Most orientations are not unique. For example: $\boldsymbol{R}(\omega, \hat{\boldsymbol{t}}) = \boldsymbol{R}((\omega + 2\pi), \hat{\boldsymbol{t}})$.
  - We are only concerned with unique crystal orientations. A set of all unique orientations is a *fundamental region* of orientation space.



    - Any orientation that is outside the fundamental region has an equivalent rotation inside the fundamental region and can be mapped to equivalent orientation.
    - Crystal symmetry reduces the size of the fundamental region orientation of a crystal type.
  - Similarly to how we express field quantities (like stress) as a function of position, we can also express quantities as a function of crystal orientation over orientation space.
  - The most common quantity expressed over orientation space is the orientation distribution function (ODF) $A(\boldsymbol{R})$. The ODF is defined:

$$v_f(\boldsymbol{R}) = A(\boldsymbol{R}) dV_{OS} \tag{40}$$

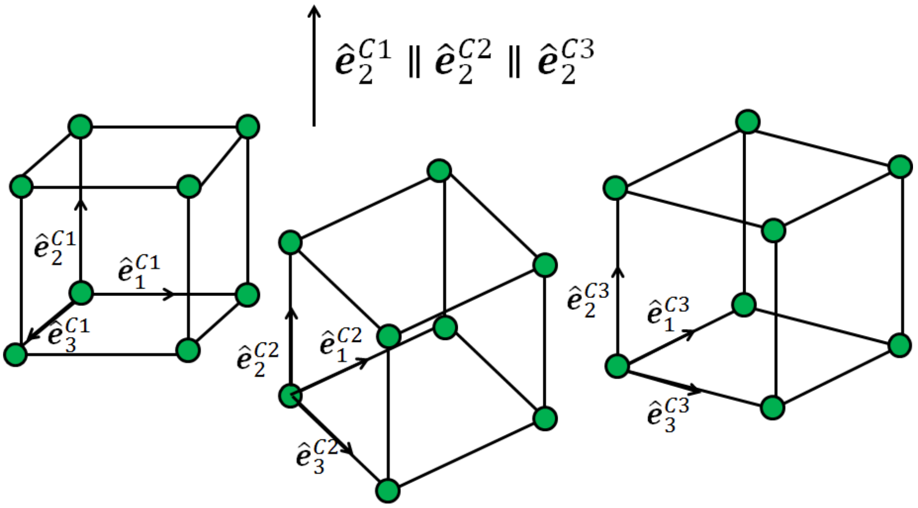
where v_f is the volume fraction of crystal with orientation $\boldsymbol{R}$ and dV_{OS} is a differential volume of orientation space.



- The ODF is normalized such that:

$$\int_{FR} A(\boldsymbol{R})dV_{OS} = 1 \tag{41}$$

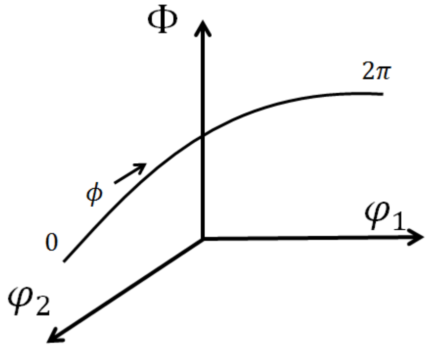
- Fibers of Orientation:
  - There exist an infinite number of orientations which can share a common crystal direction position in the external coordinate system.



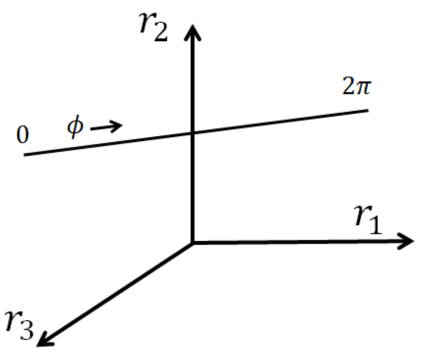
  - These sets of orientations are referred to as *fibers* of orientation. A fiber of orientations $\boldsymbol{R}(\phi)$ satisfies the relationship:

$$v_i' = R_{ij}(\phi)v_j^* \tag{42}$$

where ϕ parameterizes the angle along the fiber and $\boldsymbol{v}^*$ is a set of crystal directions expressed in different coordinate system. ***Very important to note the difference of how these fibers of orientation arise, as opposed to a single coordinate transformation.



Fibers of orientation in expressed in Euler angles are generally not straight lines



Fibers of orientation in Rodrigues space are always straight lines

- The components of a vector $\boldsymbol{v}$ expressed in the crystal $\boldsymbol{v}^C$ and sample $\boldsymbol{v}^S$ coordinate systems can be used to build a fiber of orientations (expressed as Rodrigues vectors $\boldsymbol{r}^{S,C}$). The formula is given by (note that $\boldsymbol{v}$ must be a unit vector):

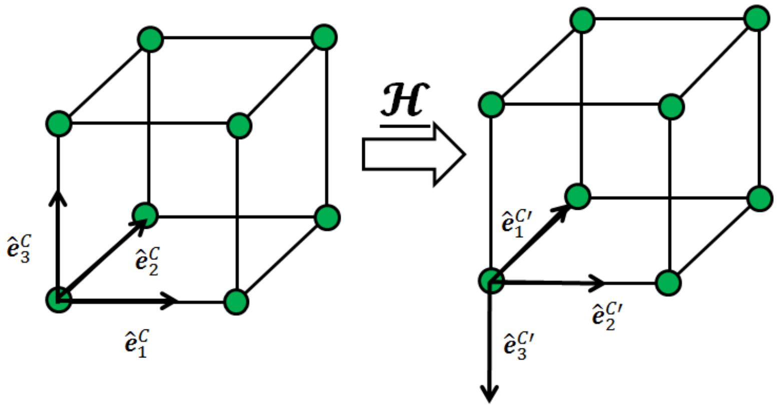
$$r_i^{S,C} = \frac{\epsilon_{ijk} v_j^C v_k^S + tan(\frac{\phi}{2})(v_i^C + v_i^S)}{1 + v_l^C \cdot v_l^S} \tag{43}$$

2.3 Symmetry

- As mentioned, all crystals have *translational* symmetry due to the periodicity of the lattice. If f describes the crystal

$$f(\boldsymbol{x} + u\boldsymbol{a_1} + v\boldsymbol{a_2} + w\boldsymbol{a_3}) = f(\boldsymbol{x}) \tag{44}$$

- Most crystals have *rotational* symmetry. We define $\boldsymbol{H}$ as a coordinate transformation which leaves all physical quantities associated with the lattice unchanged.



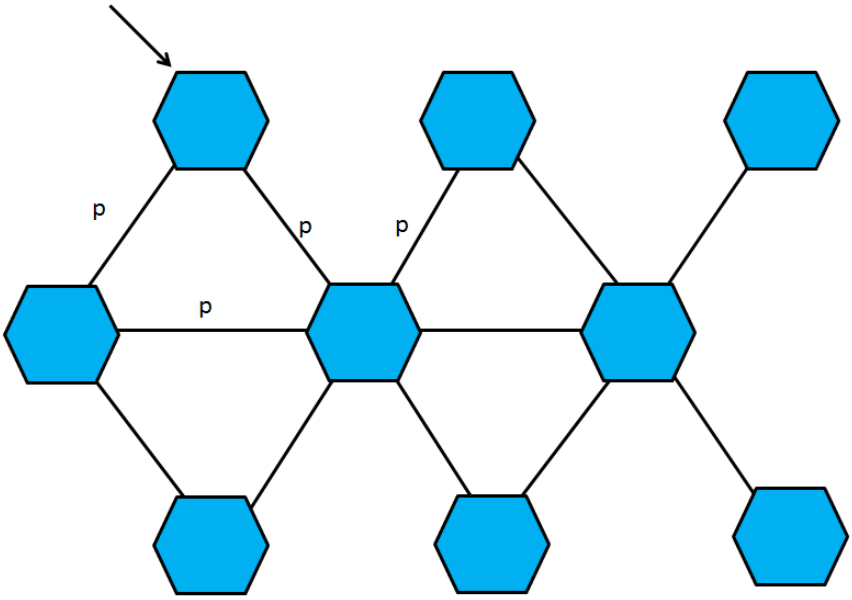
$$\hat{\boldsymbol{e}}_{\boldsymbol{i}}^{C'} = H_{ij}\hat{\boldsymbol{e}}_{\boldsymbol{j}}^{C} \tag{45}$$

$$f(x_i\hat{\boldsymbol{e}}_{\boldsymbol{i}}^{C'}) = f(x_i\hat{\boldsymbol{e}}_{\boldsymbol{i}}^{C}) \tag{46}$$

  - Note: the components of both vectors are equivalent.

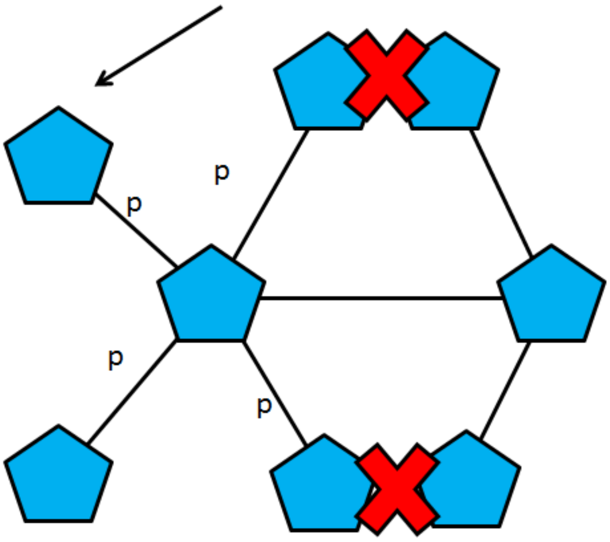
- The periodicity of the lattice places restrictions on the possible rotation symmetries. It can be shown that crystal can only have 1, 2, 3, 4, and 6 - fold symmetry.
  - Since a crystal if periodic, if a crystal has an axis about which the crystal has n-fold symmetry, this axis must also be periodic. Only, 1, 2, 3, 4, and 6 - fold symmetry axes can be periodically arranged.

A hexagon stands for a 6-fold rotation axis



6-fold axes can be periodically arranged such that every 6-fold axis, has 6 symmetrically equivalent axes a distance p away

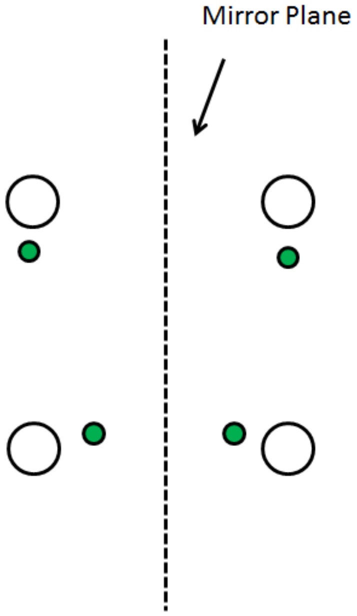
Similarly, a pentagon stands for a 5-fold rotation axis



5-fold axes can NOT be periodically arranged so that every axis has 5 symmetrically equivalent axes a distance p away

- Crystal can also have *mirror* symmetry

- If a crystal has mirror symmetry, lattice points can be 'reflected' across a mirror plane and the lattice remains unchanged.

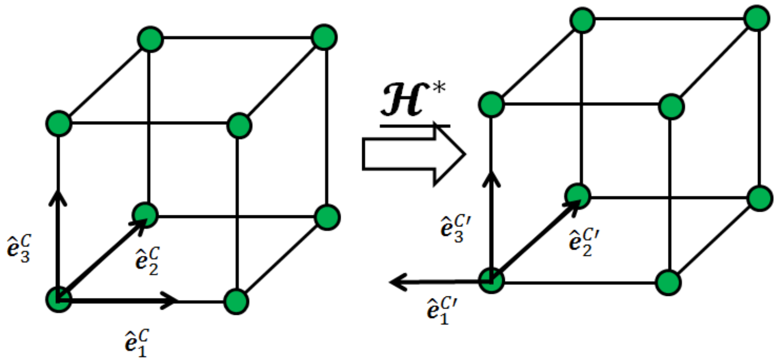


The crystal can be 'reflected' across the mirror plane

- This can be equivalently thought of as a coordinate transformation $\boldsymbol{H}^*$ from a right to a left handed coordinate system and vice versa which leaves all physical quantities associated with the lattice unchanged.

$$\hat{\boldsymbol{e}}_{\boldsymbol{i}}^{C'} = H^*_{ij}\hat{\boldsymbol{e}}_{\boldsymbol{j}}^{C} \tag{47}$$

$$f(x_i\hat{\boldsymbol{e}}_{\boldsymbol{i}}^{C'}) = f(x_i\hat{\boldsymbol{e}}_{\boldsymbol{i}}^{C}) \tag{48}$$



- As an example, $\boldsymbol{H}^*$ in which $\hat{\boldsymbol{e}}_{\boldsymbol{1}}^{C}$ and $\hat{\boldsymbol{e}}_{\boldsymbol{1}}^{C'}$ are facing opposite directions ($\hat{\boldsymbol{e}}_{\boldsymbol{1}}^{C'} \cdot \hat{\boldsymbol{e}}_{\boldsymbol{1}}^{C} = -1$)

$$\boldsymbol{H}^* = \hat{\boldsymbol{e}}_{\boldsymbol{i}}^{C'} \cdot \hat{\boldsymbol{e}}_{\boldsymbol{j}}^{C} \begin{bmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \tag{49}$$

- The existence of rotational and mirror symmetry has implications for the thermo-mechanical response of the crystal, notably the thermal expansion, elastic moduli, and yield behavior.

- Symmetry and the thermal expansion tensor
  - As a first example, we'll look at the thermal expansion of a crystal. Thermal expansion is a symmetric tensor (6 independent coefficients) which produces strain as the temperature (ΔT) in a material is changed.

$$\boldsymbol{\varepsilon} = \boldsymbol{\alpha} \Delta T \tag{50}$$

  - Following the previous the discussion, the coefficient of thermal expansion must satisfy the relation:

$$\boldsymbol{\alpha} = \boldsymbol{H} \boldsymbol{\alpha} \boldsymbol{H}^T \tag{51}$$

  - By analyzing the effects of applying rotational and mirror symmetries, we can reduce the number of independent coefficients necessary to describe the tensor.
  - For example, we may find that $\alpha_{13} = -\alpha_{13}$, therefore α_{13} must be zero. We may also find that $\alpha_{11} = \alpha_{12}$.
  - For example cubic materials only have 1 independent coefficient of thermal expansion, while hexagonal materials only have 2.

- Symmetry and the elastic stiffness tensor:
  - Recalling the general form of Hooke's Law

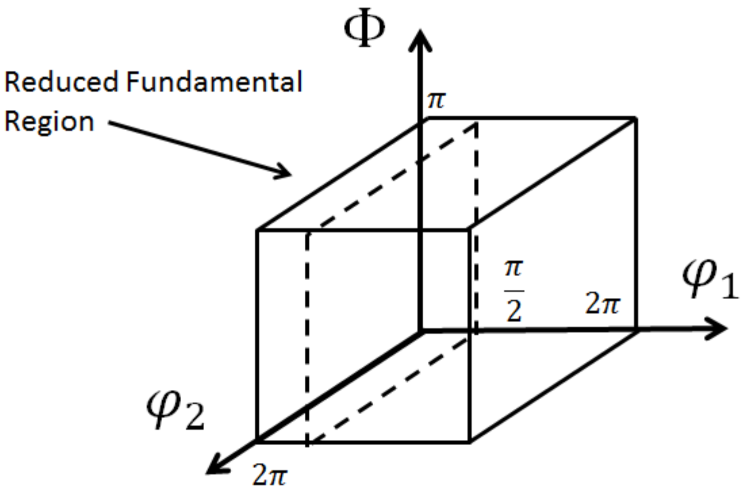
$$\sigma_{ij} = C_{ijkl} \varepsilon_{kl} \tag{52}$$

    where σ_{ij} is the Cauchy stress, C_{ijkl} is the elastic stiffness tensor, and ε_{kl} is the infinitesimal strain tensor.
  - Mechanics gets the numbers of independent constants down to 21 from 81(symmetry of stress, strain, existence of strain energy - symmetry of C_{ij}) so for triclinic materials there are 21.
  - Through similar symmetry arguments, we can find:

$$C_{ijkl} = H_{im} H_{jn} H_{ko} H_{lp} C_{mnop} \tag{53}$$

    and reduce the number of constants. A table will be provided relating the lattice types to different numbers of elastic constants.

- Symmetry and the reduction of fundamental region size:
  - As we discussed, the fundamental region is the region of orientation space which describes all unique crystallographic orientations.
  - Crystal symmetry reduces the size of the fundamental region of orientations because some orientations are symmetrically equivalent, and therefore not unique.
  - As an example if the ($\hat{\boldsymbol{e}}^3$) direction in the Bunge convention is a 4 fold rotation axis, the extent of the fundamental region along φ_1 will be reduced from 2π to $\frac{\pi}{2}$.



- **Note that the planes which reduce the size of the fundamental region of Euler Angles are not always flat.
- One of the benefits of the Rodrigues vector parameterization is that these symmetry planes are always flat in Rodrigues space.
- The planes are described by the equation:

$$\boldsymbol{r} \cdot \boldsymbol{\hat{t}_{sym}} = \tan(\frac{\omega_{sym}}{4}) \tag{54}$$

  where $\boldsymbol{\hat{t}_{sym}}$ and ω_{sym} are the axis and angle of a symmetric rotation $\boldsymbol{R_{sym}}$.
- For example, if a 120° rotation about [111] produces a symmetrically equivalent orientation, the planes which reduces the size of the fundamental region is normal to [111] and intersects, $\boldsymbol{r} = \tan(120/4)[\frac{1}{\sqrt{3}}\frac{1}{\sqrt{3}}\frac{1}{\sqrt{3}}]$ and $-\boldsymbol{r} = \tan(120/4)[\frac{1}{\sqrt{3}}\frac{1}{\sqrt{3}}\frac{1}{\sqrt{3}}]$.

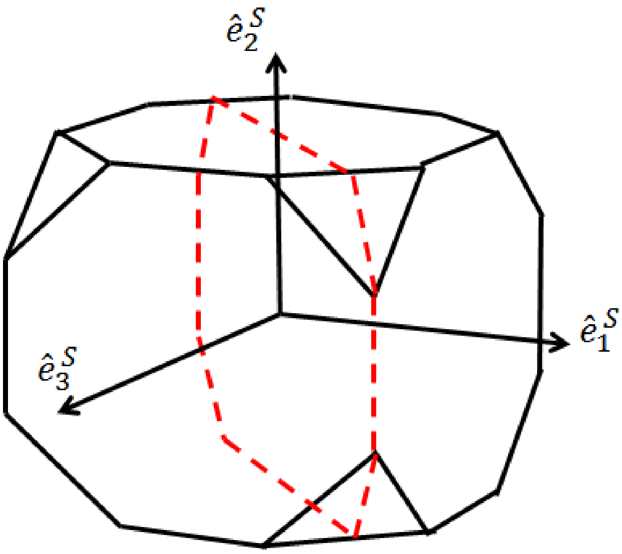
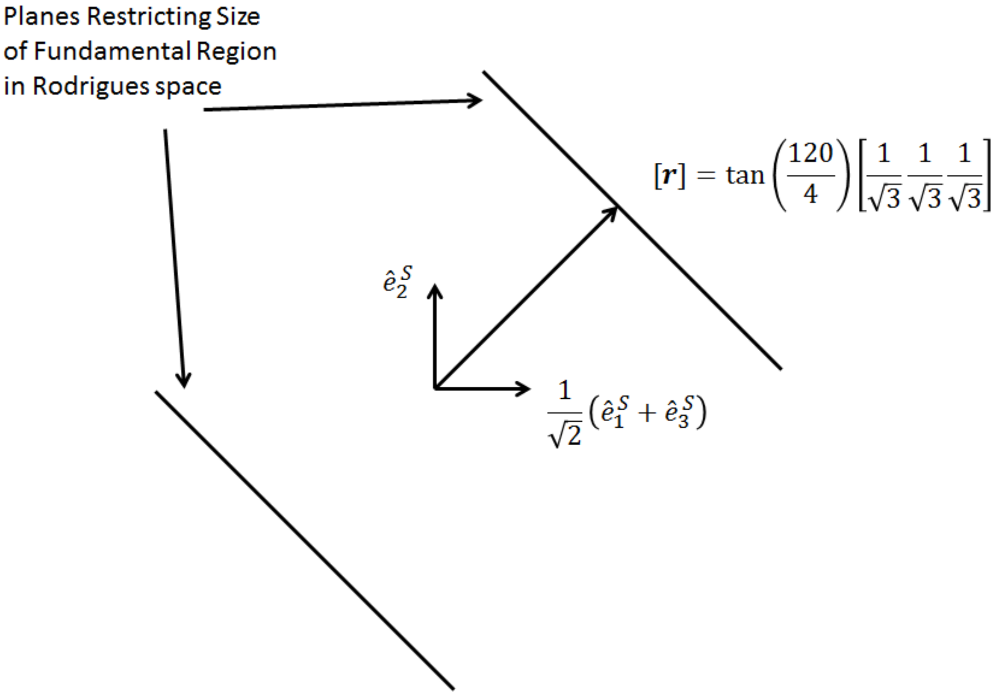


Figure 2: Plane of the cubic fundamental region being examined marked in red.

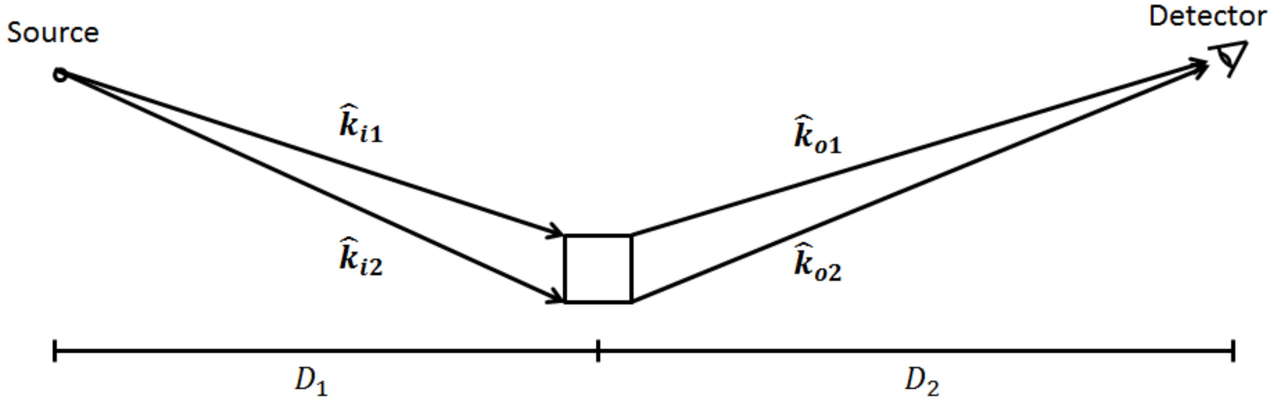


- See A. Heinz and P. Neumann (Acta. Crys., 780-789, 1991), for derivations of fundamental regions of different crystal types in Rodrigues space and pictures of what these fundamental regions look like.

3 Elements of Bragg Diffraction

3.1 X-rays and Waves

- X-rays are a form of electro-magnetic radiation. The wave nature of the X-rays allows the scattering from different atoms in a crystal to produce interference patterns that we use to study the crystal.
- In this course we will be treating X-rays as traveling plane waves (even inside the crystal). To do this, we must assume that:
    - The diffracting crystal is far away from the X-ray source (distance to source (D_1) $\gg$ source size) and our detector is far away from the diffracting crystals (detector distance (D_2) $\gg$ diffracting object size). In Figure 3, we see that as D_1 and D_2 increase, the direction of propagation of all X-rays to and from the sample become equivalent.



As D_1 and D_2 increase, the direction of propagation from the source to different parts of the sample become equivalent ($\hat{k}_{i1} \cong \hat{k}_{i2}$), and the direction of propagation waves emitted from different portions of the sample towards a single observation point become equivalent ($\hat{k}_{o1} \cong \hat{k}_{o2}$).

Figure 3: We will always assume we are very far away from our X-ray source and that our detector is far away from our sample.

-
    - The interaction of the X-ray with the crystal is weak, so that wavelength and direction of propagation of the X-ray does not appreciably change as it enters and exits the crystal.
- As quick refresher about waves in general and electromagnetic waves:
    - X-rays are a form of electromagnetic radiation. Eletromagnetic radiation are electric $\boldsymbol{E}$ and magnetic fields $\boldsymbol{B}$ described by propagating waves.
    - In this course, we will be concerned with how the electric field of the X-ray interacts with the sample.
    - A particle with charge Q experiences a force $\boldsymbol{F}$ in an electric field equivalent to:

$$\boldsymbol{F} = Q\boldsymbol{E} \tag{55}$$

  - In vacuum (or in materials with no free charge or current), the solutions to Maxwell's equations are traveling plane waves. (See Griffith's Intro to Electrodynamics pg 375) Therefore, X-rays (as a form of electromagnetic radiation) can be modeled as plane waves.
  - The general form of a plane wave is:

$$\Psi = A\cos(\boldsymbol{k}\cdot\boldsymbol{x} - 2\pi\nu t + \phi) \tag{56}$$

    where A is the wave amplitude, $\boldsymbol{k}$ is the wave vector, ν is the frequency of the wave, and ϕ is a phase shift.
  - The wave vector $\boldsymbol{k}$ is equal to

$$\boldsymbol{k} = \frac{2\pi}{\lambda}\hat{\boldsymbol{k}} \tag{57}$$

  - λ is the wave length of the wave and $\hat{\boldsymbol{k}}$ is the direction of propagation.
  - However, it is much easier to do calculations using a complex description of the wave.

$$\Psi = Ae^{i(\boldsymbol{k}\cdot\boldsymbol{x}-2\pi\nu t)} = A(\cos(\boldsymbol{k}\cdot\boldsymbol{x} - 2\pi\nu t + \phi) + i\sin(\boldsymbol{k}\cdot\boldsymbol{x} - 2\pi\nu t + \phi)) \tag{58}$$

    while remembering only the real portion of this description describes our wave.
  - For electromagnetic radiation the frequency of the wave ν and the wavelength are related:

$$\lambda\nu = c \tag{59}$$

    where c is the speed of light.
  - The electric field $\boldsymbol{E}$ and the magnetic field $\boldsymbol{B}$ associated with the radiation are perpendicular to each other and the direction of propagation $\hat{\boldsymbol{k}}$.
  - Since X-rays are often described by their energy, the energy (En) of a photon is given by:

$$En = h\nu \tag{60}$$

    where h is Planck's constant.

- Measurement and Intensity
  - We generally can not measure the electric field of an X-ray beam. Instead we measure the *Intensity* I of the beam.
  - The intensity of the beam is proportional to the amplitude squared of the electric field.

$$I \propto ||E||^2 = \boldsymbol{E}\cdot\boldsymbol{E}^* \tag{61}$$

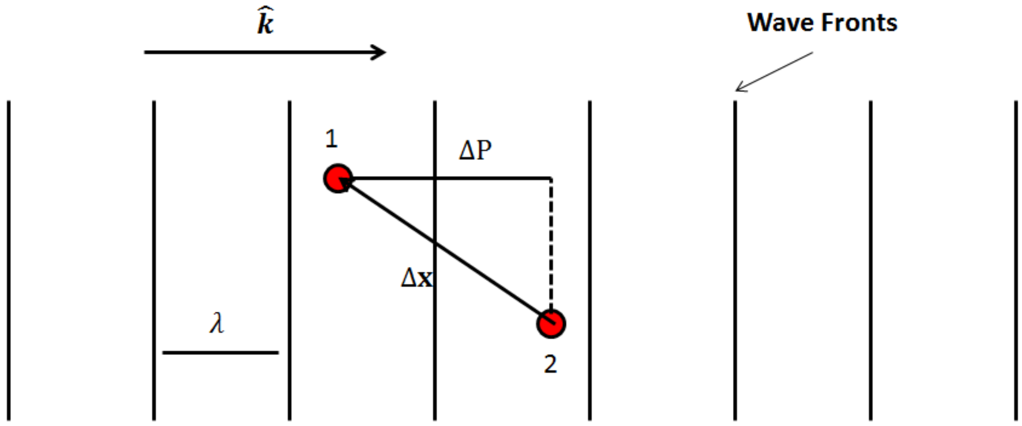
  - We measure the intensity of X-ray by counting the number of photons with energy En that hit out detector per second.

$$I = \#photons * \frac{En}{photon}/s \tag{62}$$

- Interference:
  - Due to the superposition principle, E&M waves that occupy the same space *interfere* one another
  - The interference of waves that have different frequencies is time dependent, and generally averages out very quickly.
  - However, the interference of waves that have the same frequency (and wavelength) is not time dependent, and produce diffraction patterns that we can measure.
    - ∗ From this point on, we will neglect the frequency portion of our wave description since we are only concerned with waves of the same wavelength which produce time independent interference.
  - If the waves are of the same frequency, only the relative difference in phase effect the amplitude of the resultant wave.

$$\Psi = \Psi_1 + \Psi_2 = Ae^{i(\boldsymbol{k}\cdot\boldsymbol{x})} + Ae^{i(\boldsymbol{k}\cdot\boldsymbol{x}+\phi)} = A(1+e^{i\phi})(e^{i(\boldsymbol{k}\cdot\boldsymbol{x})}) \tag{63}$$

  - As the phase shift ϕ varies from 0 to 2π, the interference shifts from fully constructive ($\phi = 0$), to fully destructive ($\phi = \pi$), back to fully constructive ($\phi = 2\pi$).
  - The phase shift of a plane wave observed between points in space that are a vector $\Delta\boldsymbol{x}$ apart is only related to the path length difference that the waves have traveled.

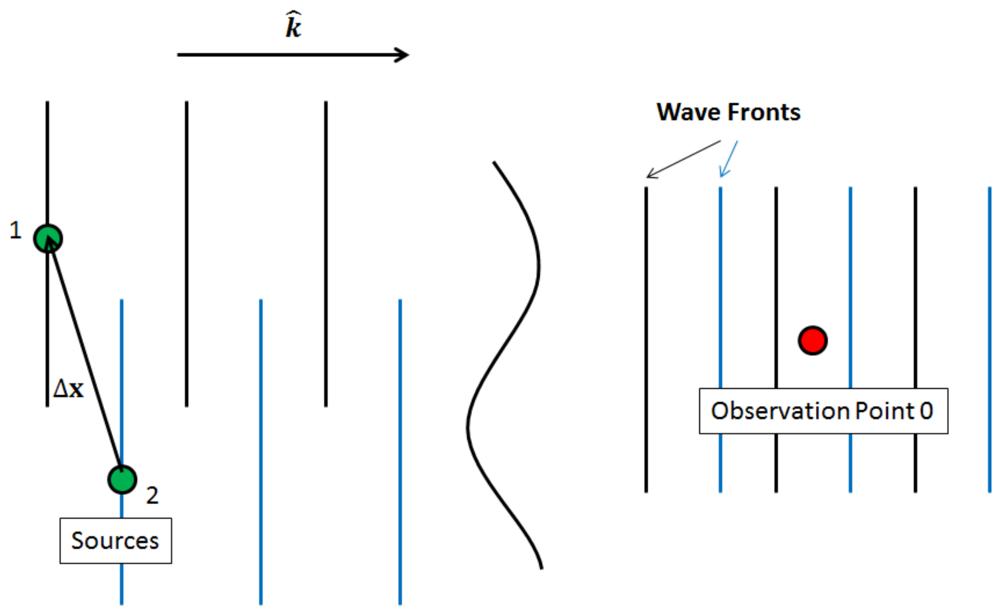


The apparent phase shift of the plane wave when it hits object 2 with respect to object 1 (a vector **Δx** apart) is $\boldsymbol{k} \cdot (-\Delta\mathbf{x})$ (note the vector points from 2 to 1)

- If we express the phase shift in terms of the path length difference along the direction of propagation (ΔP)

$$\phi = \frac{2\pi}{\lambda}\Delta P = \frac{2\pi}{\lambda}\hat{\boldsymbol{k}} \cdot -\Delta\boldsymbol{x} = -\boldsymbol{k}\cdot\Delta\boldsymbol{x} \tag{64}$$

  - Note that the vector $\Delta\boldsymbol{x}$ points from 2 to 1.
  - We can see that if ΔP is a integer (m) multiple of λ, we will get fully constructive interference ($e^{i2m\pi} = 1$).
  - Similarly, if plane waves with wave vector $\boldsymbol{k}$ are emitted from 2 different sources, and observed at a point O.



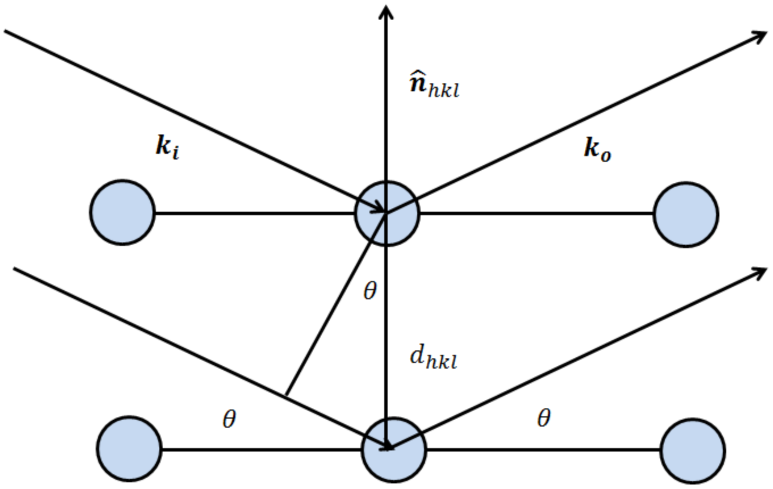
The apparent phase shift of the plane wave from source 2 with respect to source 1 observed at pt O is $\boldsymbol{k} \cdot \Delta\mathbf{x}$ (note the vector points from 2 to 1)

we see that the phase shift is equal to

$$\phi = \boldsymbol{k} \cdot \Delta\boldsymbol{x} \tag{65}$$

3.2 Bragg's Law

- With the basics out of the way, we can now introduce the simplest diffraction model and derive Bragg's law. A good, simple reference for Bragg's law and a presentation of very basic diffraction concepts is [3].



- We wish to know at what angle (θ, usually called the Bragg angle) must a set of lattice planes be oriented with respect to an incoming X-ray beam $\boldsymbol{k_i}$ in order to measure appreciable diffracted intensity.
- We will assume that a set of lattice planes 'reflects' X-rays ($\boldsymbol{k_o}$) at the same angle as the incoming beam.

- In addition, the scattering is *elastic* (no change in X-ray energy) so the wave lengths of the incoming and diffracted beams are the same.
- The lattice planes are spaced a distance d apart from one another.
- From the previous section, we know that the path length difference of the 'reflected' beams must be equal to $m\lambda$.
- In addition, we can see from our sketch that the path length difference of X-rays reflected from two adjacent lattice planes is equal to:

$$\Delta P = 2d\sin(\theta). \tag{66}$$

- So in total, we find the familiar Bragg's Law:

$$m\lambda = 2d\sin(\theta). \tag{67}$$

- If the sample is illuminated by monochromatic X-rays, we can drop the integer m.

$$\lambda = 2d\sin(\theta). \tag{68}$$

- Some notes about Bragg's Law:
  - The the angle between $\boldsymbol{k_i}$ and $\boldsymbol{k_o}$ is 2θ. This is the angle which is typically measured in an experiment.
  - In the derivation, we assumed that we were able to rotate our crystal about an axis which is perpendicular to $\boldsymbol{k_i}$ and $\boldsymbol{n_{hkl}}$. Bragg's law isn't very useful for predicting when diffraction will occur when this isn't possible.
  - For a given crystal orientation multiple wavelength of X-rays can be diffracted. When using a crystal to monochromate (select one wavelength from) a polychromatic beam, the undesired wavelengths are called *harmonic contamination*

3.3 X-Ray Absorption

- As an X-ray beam travels through matter, the intensity of the beam (I) is attenuated either by scattering of X-ray or absorption.
- A simple model for absorption is that the change in intensity per distance traveled ($\frac{dI}{dx}$) is proportional to the intensity of the beam:

$$\frac{dI}{dx} = -\mu I = -\frac{\mu}{\rho}\rho I \tag{69}$$

- where μ is the X-ray absorption coefficient and ρ is the density of the material.
- The solution to the above equation is a decaying exponential.

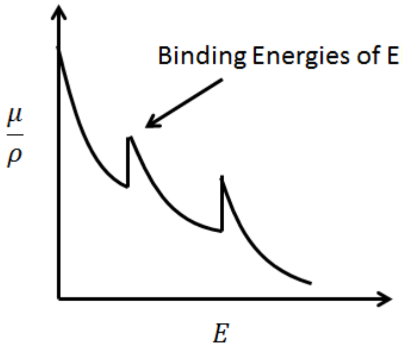
$$I = I_0 e^{(-\mu x)} \tag{70}$$

- The constant μ varies with X-ray energy and material with the approximate relation:

$$\frac{\mu}{\rho} \propto \frac{Z^4}{E^3} \tag{71}$$

  where Z is the atomic number and E is the X-ray energy. So, if we want to penetrate further into materials, we need to increase our X-ray energy. This is why the *High Energy X-rays* that are available at some synchrotron sources are so valuable.

- *It should be noted that μ increases rapidly near the binding energies of different electron shells of an atom. A typical $\frac{\mu}{\rho}$ chart:



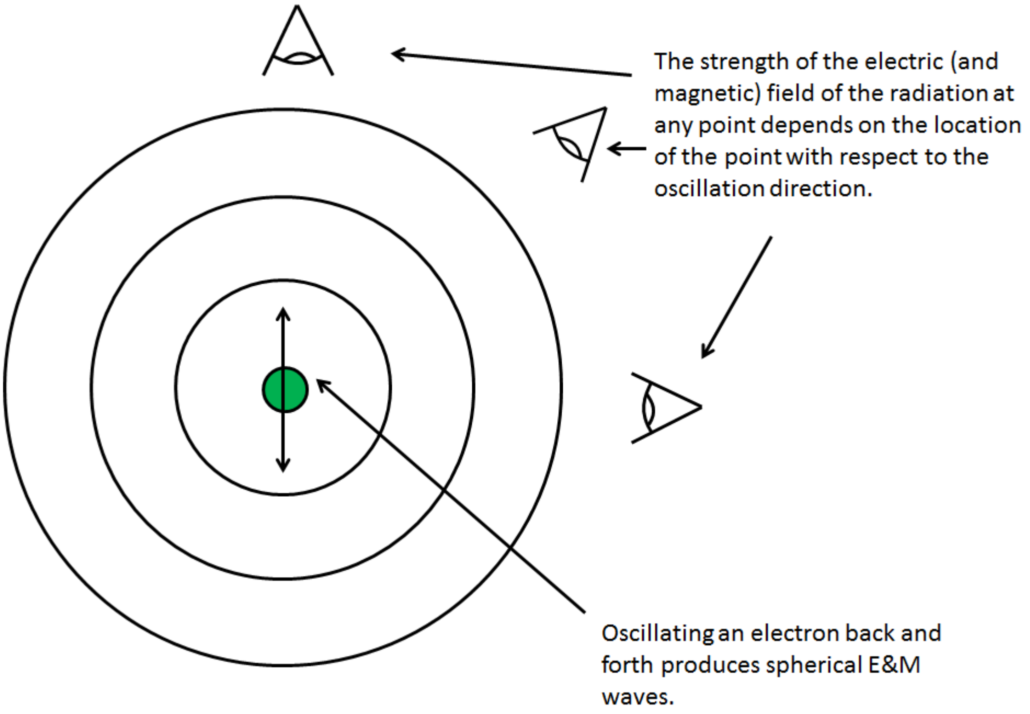
- Values of $\frac{\mu}{\rho}$ versus X-ray energy can be found on the NIST website.

4 The Laue Equations and The Rotating Crystal Experiment

4.1 Scattering from an Electron

- Our first assumption is that we are under kinematic diffraction conditions (defined in detail in a later section). We will start, by looking at the scattering from a single electron. The derivations will be neglected, but if you are interested, they can be found in [4] page 444-454 or [5] page 349-353.

- If an electron at the origin is excited by an oscillating electric field, wave vector $\boldsymbol{k_i}$ and frequency ω_0 (similar to a forced harmonic oscillator, but instead of applying an oscillating force on a spring, we are applying an oscillating electric field on a charge), a spherical wave is emitted.



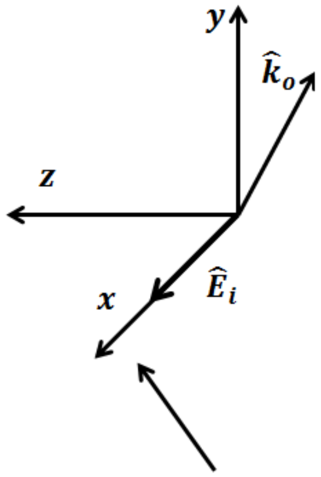
- The magnitude of the electric field emitted $\boldsymbol{E_o}$ by the electron is:

$$||\boldsymbol{E_o}(\boldsymbol{x})|| = \frac{A}{||\boldsymbol{x}||} e^{i(||\boldsymbol{k_o}||*||\boldsymbol{x}||-\omega_0 t+\phi)} P \tag{72}$$

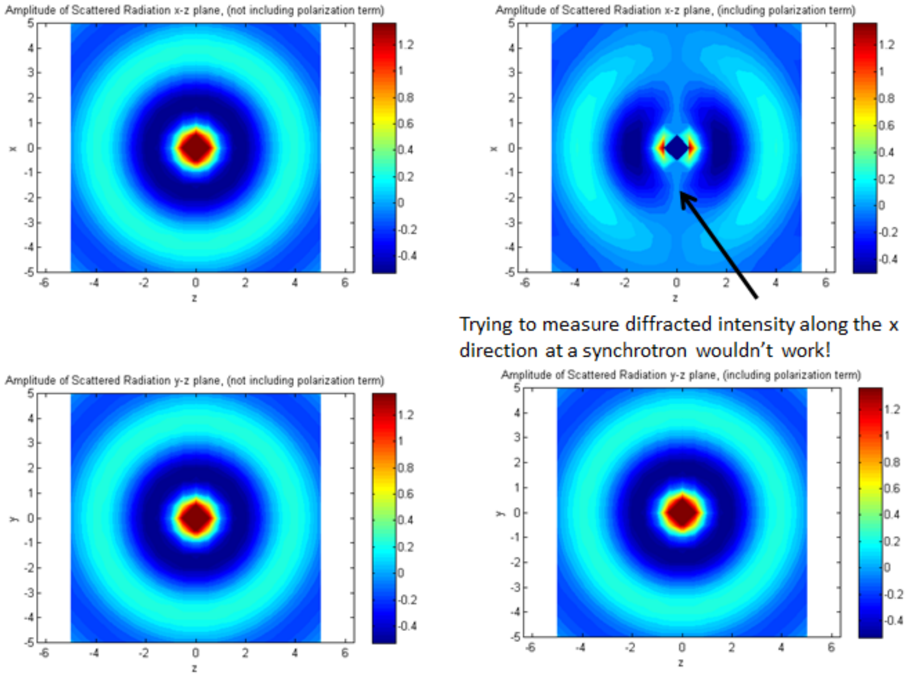
  where $\boldsymbol{x}$ is the distance from the origin, A is a constant (we will define A as $||\boldsymbol{E_i}||A_0$, and P is the polarization factor. (A_0 is constant found when classically deriving the scattering from an electron). The polarization factor is given by:

$$P = 1 - |\hat{\boldsymbol{E}}_{\boldsymbol{i}} \cdot \hat{\boldsymbol{k}}_{\boldsymbol{o}}| \tag{73}$$

- At a synchrotron, the polarization of the incoming X-ray beam ($\hat{\boldsymbol{E}}_{\boldsymbol{i}}$ (which way the electric field of the incoming beam is pointing) is oriented towards the center of the ring. This means the polarization term is important for some experiments. Below is a picture of the amplitude of the scattered radiation at synchrotron:

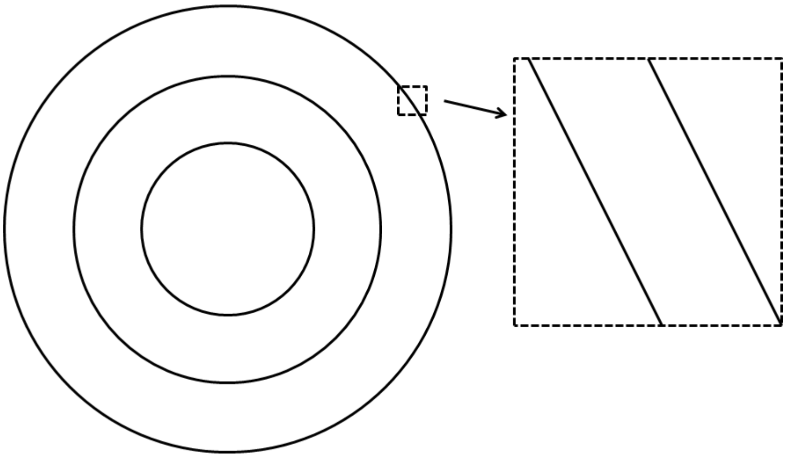


x points towards the ring center



Trying to measure diffracted intensity along the x direction at a synchrotron wouldn't work!

- We can see that polarization does not effect scattering in the Y-Z plane, which is why diffraction experiments are typically conducted in this plane. However, if we tried measuring diffracted intensity near $\boldsymbol{x}$, nothing would be measured!
- Some things to note:
  - We will generally be very far away from the scattering electrons, so the regions of the spherical waves we observe can be approximated as plane waves.

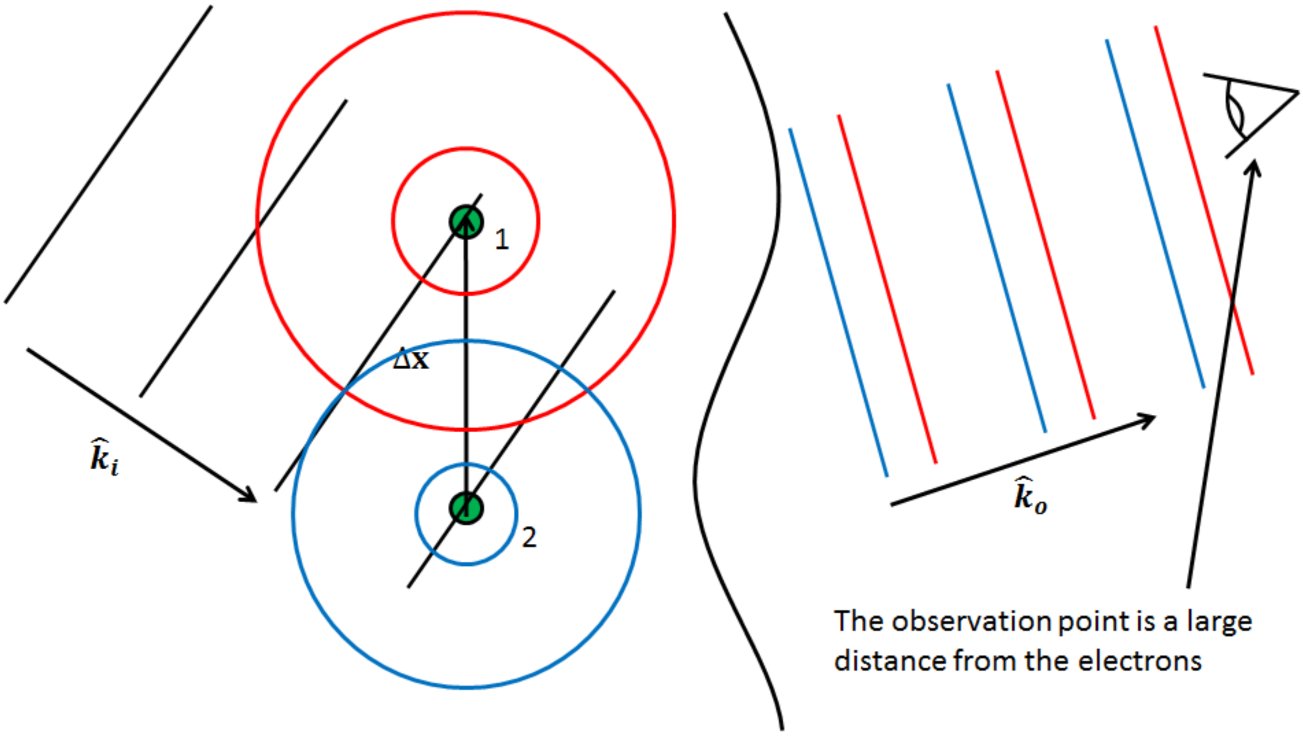


  - The phase shift for a high frequency oscillating field, is π so the outgoing electric field is exactly out of phase with the incoming field.
  - The magnitude of wave vector and frequency of the outgoing and incoming electric fields are the same so the scattering is *elastic*. This places a very important constrain on the scattering.

$$||\boldsymbol{k}_i|| = ||\boldsymbol{k}_o|| \tag{74}$$

4.2 The Scattering Vector

- To introduce the scattering vectors, lets look at the interference from two electrons, separated by a vector $\Delta\boldsymbol{x}$, and both excited by an incoming X-ray beam with wave vector $\boldsymbol{k_i}$. We'll assume that we are far enough away ($\boldsymbol{x}$) that we can model the scattered radiation from the two electron as plane waves.



The phase shift difference of the scattered X-rays from the two electrons is due to the incoming beam reaching electron 1 first, AND the extra distance the waves from electron 2 must travel to reach an observation point in the $\hat{k}_o$ direction

- The total scattered amplitude we see is:

$$A_{TOT} = \frac{A}{||\boldsymbol{x}||}e^{i(\boldsymbol{k_o}\cdot\boldsymbol{x})} + \frac{A}{||\boldsymbol{x}+\Delta\boldsymbol{x}||}e^{i(\boldsymbol{k_o}\cdot(\boldsymbol{x}+\Delta\boldsymbol{x})+\phi)} \tag{75}$$

- Since we are far away from the sample:

$$\boldsymbol{x}+\Delta\boldsymbol{x} \approx \boldsymbol{x} \tag{76}$$

- This simplifies things quite a bit:

$$A_{TOT} = \frac{A}{||\boldsymbol{x}||}e^{i(\boldsymbol{k_o}\cdot\boldsymbol{x})}(1+e^{i(\phi)}) \tag{77}$$

- Now, we just need to find the phase shift ϕ.
- Looking at figure, we can see that the phase shift of the incoming beam from the first to second electrons is: (Remind yourself from our earlier notes if necessary)

$$\phi_1 = \boldsymbol{k_i}\cdot(-\Delta\boldsymbol{x}) \tag{78}$$

while the phase shift between the scattered beams is:

$$\phi_2 = (\boldsymbol{k_o} \cdot (\Delta \boldsymbol{x})) \tag{79}$$

- The total phase shift between the two scattered beams is the sum of these two phase shifts:

$$\phi = \phi_1 + \phi_2 = \boldsymbol{k_i} \cdot (-\Delta \boldsymbol{x}) + (\boldsymbol{k_o} \cdot \Delta \boldsymbol{x}) = (\boldsymbol{k_o} - \boldsymbol{k_i}) \cdot \Delta \boldsymbol{x} \tag{80}$$

- We will define the *scattering vector* $\boldsymbol{q}$ as:

$$\boldsymbol{q} = \boldsymbol{k_o} - \boldsymbol{k_i} \tag{81}$$

which allows us to simplify our equation for our total scattered amplitude to:

$$A_{TOT} = \frac{A}{||\boldsymbol{x}||} e^{i(\boldsymbol{k_o} \cdot \boldsymbol{x})} (1 + e^{i(\boldsymbol{q} \cdot \Delta \boldsymbol{x})}) \tag{82}$$

- This easily generalized to more than one electron, where we find:

$$A_{TOT} = \frac{A}{||\boldsymbol{x}||} e^{i(\boldsymbol{k_o} \cdot \boldsymbol{x})} (1 + \sum_{j=1}^{nume-} e^{i(\boldsymbol{q} \cdot \Delta \boldsymbol{x}_j)}) \tag{83}$$

4.3 Scattering from an Atom

- To determine the scattering from an electron, we will smear the charge of the electron out into a charge density.
- The scattered amplitude dA from a volume dV with charge density ρ_{ch} is equal to:

$$dA_{ATOM} = A \rho_{ch} dV \tag{84}$$

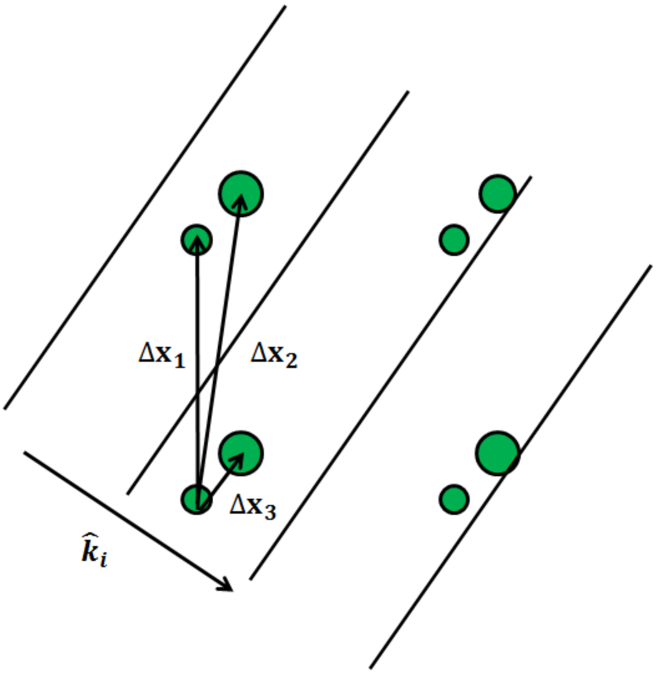
- Knowing that the phase shift at the point of observation between different scattering entities is $\boldsymbol{q} \cdot \Delta \boldsymbol{x}$, the scattered amplitude (f) from an atom is found by integrating the contributions from the charge density at all points in the atom:

$$f(\boldsymbol{q}) = \int_{ATOM} \rho_{ch}(\Delta \boldsymbol{x}) e^{i(\boldsymbol{q} \cdot \Delta \boldsymbol{x})} dV \tag{85}$$

- $f(\boldsymbol{q})$ is referred to as the *atomic scattering factor*. Note its dependence on $\boldsymbol{q}$. In theory, if the charge density is known, $f(\boldsymbol{q})$ can be calculated. In reality, the charge density is rarely known and $f(\boldsymbol{q})$ is measured. $f(\boldsymbol{q})$ can be found in the International Tables of Crystallography or the yellow X-ray Data Booklet (http://xdb.lbl.gov/).

4.4 Scattering from a Crystal (Diffraction)

- To find the scattered amplitude of a crystal at an observation point $\boldsymbol{x}$, we simply add together the amplitudes from every atom in the crystal, while taking into account the corresponding phase shifts.



- We will use $\boldsymbol{\Delta x_n}$ to describe a vector from one atom OUT to another atom n. This will give us an extra minus in the derivation because of how we have defined $\boldsymbol{q}$. However, this does not affect the final result.

- If we want to examine the scattering from a crystal, we simply sum up the effects of scattering from all the different atoms in the crystal.

$$A_{TOT} = A \sum_{n}^{atoms} f_n(\boldsymbol{q}) e^{-i(\boldsymbol{q}\cdot\Delta\boldsymbol{x}_n)} \tag{86}$$

  where we are summing over the n atoms in the crystal at positions $\Delta\boldsymbol{x}_n$. (*Note that we are neglecting the effects of the distance from source to observation point)

- Every atom position $\Delta\boldsymbol{x}_n$ can be decomposed into the position to its associated unit cell origin $\boldsymbol{X}_N$ and its position in the unit cell $\boldsymbol{z}_j$.

$$\Delta\boldsymbol{x}_n = \boldsymbol{X}_N + \boldsymbol{z}_j \tag{87}$$

- We should remember that

$$\boldsymbol{X}_N = u\boldsymbol{a}_1 + v\boldsymbol{a}_2 + w\boldsymbol{a}_3 \tag{88}$$

- If we plug equation 87 into equation 86, we get:

$$A_{TOT} = A \sum_{n}^{atoms} f_j(\boldsymbol{q}) e^{-i(\boldsymbol{q}\cdot(\boldsymbol{X}_N+\boldsymbol{z}_j))} = A \sum_{N}^{cells} \sum_{j} f_j(\boldsymbol{q}) e^{-i(\boldsymbol{q}\cdot(\boldsymbol{X}_N+\boldsymbol{z}_j))} \tag{89}$$

$$A_{TOT} = A\sum_{N}^{cells} e^{-i(\boldsymbol{q}\cdot\boldsymbol{X}_N)} \sum_{j} f_j(\boldsymbol{q}) e^{-i(\boldsymbol{q}\cdot\boldsymbol{z}_j)} \tag{90}$$

- Lets take a closer look at the first term in our summation. Inside the summation $e^{-i(\boldsymbol{q}\cdot\boldsymbol{X}_N)}$ can vary from -1 to 1. In order for the terms of the summation not to cancel each other out:

$$\boldsymbol{q}\cdot\boldsymbol{X}_N = 2\pi m \tag{91}$$

- where m is an integer. The only way this is possible is if:

$$\boldsymbol{q} = \boldsymbol{g_{hkl}} \tag{92}$$

since

$$\boldsymbol{g_{hkl}}\cdot\boldsymbol{X}_N = 2\pi(hu + kv + wl) \tag{93}$$

- Equation 92 is known as the Laue Diffraction condition. This equation is the vector form of the Bragg diffraction condition given by Bragg's law. It basically states that 'when the scattering vector is equal to a reciprocal lattice vector, diffraction occurs.
- This equation sits at the heart of what we will be doing for the rest of the course.
- We note that we don't measure the amplitude of the scattered electric field, but its intensity.

$$I(\boldsymbol{q}) = ||A_{TOT}||^2 = A^2||\sum_{N}^{cells} e^{-i(\boldsymbol{q}\cdot\boldsymbol{X}_N)}||^2||\sum_{j} f_j(\boldsymbol{q}) e^{-i(\boldsymbol{q}\cdot\boldsymbol{z}_j)}||^2 \tag{94}$$

- This equation can be further simplified, by noting that:

$$||A_{TOT}||^2 = ||\boldsymbol{E_i}||^2 A_0^2 = I_i A_0^2 \tag{95}$$

where I_i is the intensity of the incoming beam. Also, $||\sum_{N}^{cells} e^{-i(\boldsymbol{q}\cdot\boldsymbol{X}_N)}||^2$ can be analytically simplified (see Als-Neilsen pg 52):

$$||\sum_{N}^{cells} e^{-i(\boldsymbol{q}\cdot\boldsymbol{X}_N)}||^2 = Nv^*\delta(\boldsymbol{q} - \boldsymbol{g_{hkl}}) \tag{96}$$

where v^* is the volume of reciprocal lattice unit cell. This gives our final intensity of a diffraction peak as:

$$I(\boldsymbol{q}) = I_i A_o^2 N v^* ||\sum_{j} f_j(\boldsymbol{q}) e^{-i(\boldsymbol{q}\cdot\boldsymbol{x}_j)}||^2 \delta(\boldsymbol{q} - \boldsymbol{g_{hkl}}) \tag{97}$$

$$I(\boldsymbol{g_{hkl}}) = I_i A_o^2 N v^* ||\sum_{j} f_j(\boldsymbol{g_{hkl}}) e^{-i(\boldsymbol{g_{hkl}}\cdot\boldsymbol{z}_j)}||^2 \tag{98}$$

The Unit Cell Structure Factor (and Forbidden Reflections)

- Now, looking at the second term of equation 90. This term is referred to as the *unit cell structure factor* $F(\boldsymbol{q})$.

$$F(\boldsymbol{q}) = \sum_j f_j(\boldsymbol{q}) e^{-i(\boldsymbol{q}\cdot\boldsymbol{z_j})} \tag{99}$$

- Since, we just found that $\boldsymbol{q} = \boldsymbol{g_{hkl}}$ in order for appreciable diffracted intensity can be measured from the crystal, we can insert $\boldsymbol{g_{hkl}}$ into the unit cell structure factor to find the relative intensities of different reflections.
- Some structure factors for different $\boldsymbol{g_{hkl}}$ are equal to 0, and even though the Laue diffraction condition is satisfied, diffracted intensity will not be measured.
- When this happens, the corresponding reflection is referred to as *forbidden reflection*

Example: Calculating the structure factor of the (001) reciprocal lattice vector for an hcp material (2 identical atoms in the unit cell).

Our crystal basis vector components expressed in the crystal coordinate system are given by:

$$\boldsymbol{a_1^C} = \begin{bmatrix} a \\ 0 \\ 0 \end{bmatrix} \mathring{A}, \boldsymbol{a_2^C} = \begin{bmatrix} -\frac{a}{2} \\ a\frac{\sqrt{3}}{2} \\ 0 \end{bmatrix} \mathring{A}, \boldsymbol{a_3^C} = \begin{bmatrix} 0 \\ 0 \\ c \end{bmatrix} \mathring{A}$$

The atom positions are:

$$\boldsymbol{z_1} = 0\boldsymbol{a_1} + 0\boldsymbol{a_2} + 0\boldsymbol{a_3}$$

$$\boldsymbol{z_2} = \tfrac{1}{3}\boldsymbol{a_1} + \tfrac{2}{3}\boldsymbol{a_2} + \tfrac{1}{2}\boldsymbol{a_3}$$

We will assume that the atomic scattering factor ($f(\boldsymbol{q})$) is equal to 1.

So our atomic structure factor is:

$$F(\boldsymbol{g_{001}}) = \textstyle\sum_j e^{-i((0\boldsymbol{b_1}+0\boldsymbol{b_2}+1\boldsymbol{b_3})\cdot\boldsymbol{x}_j)}$$

$$F(\boldsymbol{g_{001}}) = e^{-i((1\boldsymbol{b_3})\cdot(0\boldsymbol{a_1}+0\boldsymbol{a_2}+0\boldsymbol{a_3}))} + e^{-i((1\boldsymbol{b_3})\cdot(\frac{1}{3}\boldsymbol{a_1}+\frac{2}{3}\boldsymbol{a_2}+\frac{1}{2}\boldsymbol{a_3}))}$$

Remembering that $\boldsymbol{b_3}\cdot\boldsymbol{a_1} = 0$, $\boldsymbol{b_3}\cdot\boldsymbol{a_2} = 0$, and $\boldsymbol{b_3}\cdot\boldsymbol{a_3} = 2\pi$:

$$F(\boldsymbol{g_{001}}) = e^{-i(2\pi)} + e^{-i(\pi)}$$

$$F(\boldsymbol{g_{001}}) = 1 - 1 = 0$$

$$||F(\boldsymbol{g_{001}})||^2 = 0$$

Since the unit cell structure factor is 0, this reflection is forbidden.

4.5 Ewald's Sphere

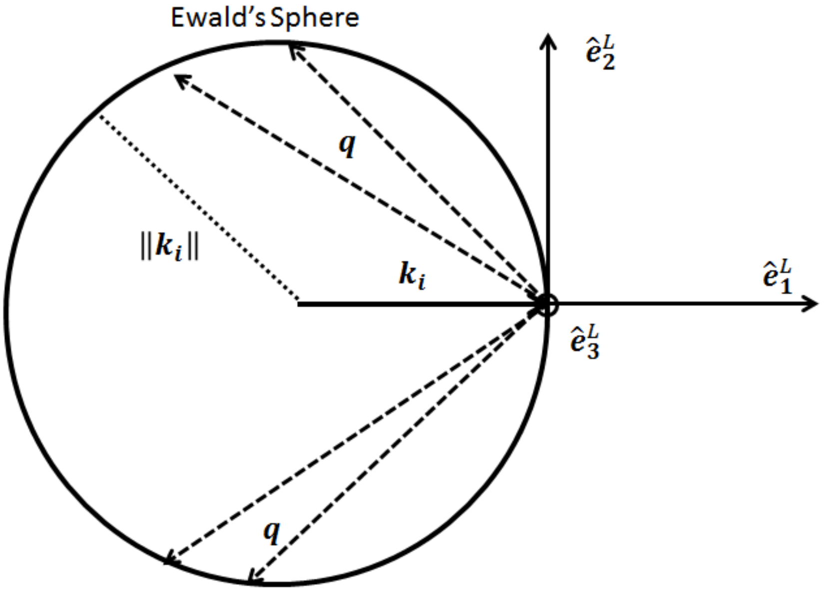
- A convenient way to visualize the diffraction condition is the Ewald Sphere construction.
- We discussed previously that the scattering we are analyzing is elastic, so:

$$||\boldsymbol{k_i}|| = ||\boldsymbol{k_o}|| \tag{100}$$

while using our definition of the scattering vector ($\boldsymbol{q} = \boldsymbol{k_o} - \boldsymbol{k_i}$), we see that:

$$||\boldsymbol{k_i}|| = ||\boldsymbol{k_i} + \boldsymbol{q}||. \tag{101}$$

- Equation 101 restricts the allowed values of $\boldsymbol{q}$ for a fixed $\boldsymbol{k_i}$.
- Graphically, if $\boldsymbol{q}$ is a vector that extends out from the origin of reciprocal space, all allowed values of $\boldsymbol{q}$ sit on a sphere of magnitude $||\boldsymbol{k_i}||$ that is centered at $-\boldsymbol{k_i}$ from the origin. Shown below is an illustration:

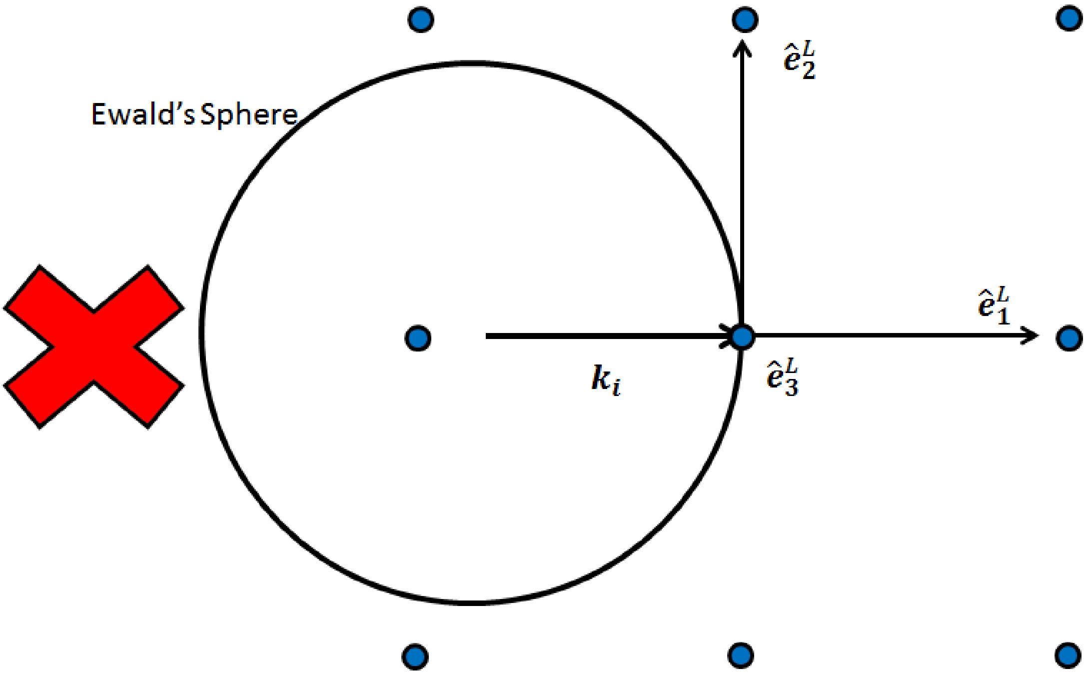


The dashed arrows, indicates possible values of $\boldsymbol{q}$ for a fixed $\boldsymbol{k_i}$. All allowed values of $\boldsymbol{q}$ lie on a sphere of radius $||\boldsymbol{k_i}||$, known as Ewald's sphere.

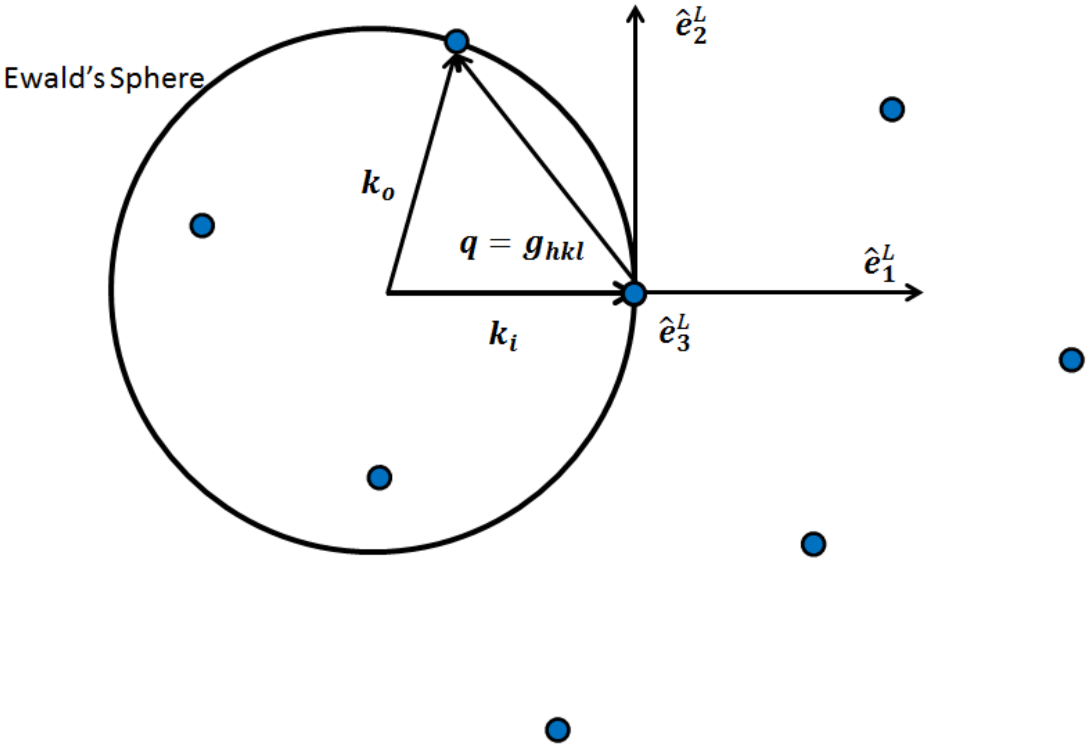
- We also know from the Laue diffraction condition ($\boldsymbol{q} = \boldsymbol{g_{hkl}}$), that the scattering vector must equal a reciprocal lattice vector for diffraction to occur. Changing equation 101 to reflect this:

$$||\boldsymbol{k_i}|| = ||\boldsymbol{k_i} + \boldsymbol{g_{hkl}}||. \tag{102}$$

- So moving back to our schematic, a reciprocal lattice vector must lie on Ewald's sphere for diffraction to occur.



Blue spheres indicate reciprocal lattice points. Since, no points are in contact with Ewald's sphere, diffraction does not occur.



A reciprocal lattice point is in contact with Ewald's sphere, so diffraction will occur.

- With Ewald's sphere we can graphically see how rotating the crystal (and the attached reciprocal lattice) will move reciprocal lattice vectors in to and out of the diffraction condition.

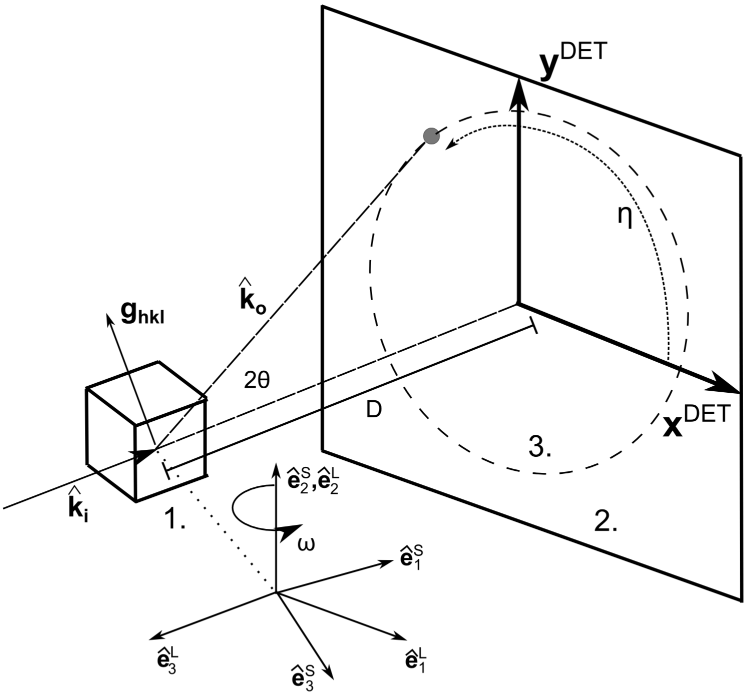
4.6 Rotating Crystal Diffraction Experiments

- As, we saw with our Ewald's sphere construction, for nearly all crystal orientations, diffraction will not occur when the crystal is merely illuminated by monochromatic X-rays.
- In order to get a reciprocal lattice vector into the diffraction condition, we must rotate the crystal so that a set of lattice planes comes into right geometry for diffraction to happen.
- The simplest way to do this is to rotate the crystal about one or more axes - the most common in our work is the use of a single axis $\hat{\boldsymbol{t}}$ (that is often perpendicular) to the incoming beam direction. This is known as a *rotating crystal diffraction experiment* and is shown schematically below.
- When we are conducting these experiments, if the crystal structure and the crystal orientation with respect to the sample is known, we can solve for the angles ω about $\hat{\boldsymbol{t}}$ about which the sample must be rotated in order for diffraction to occur.
- Returning to 102, and taking more care as to which coordinate system we are working in:

$$||\boldsymbol{k}_{\boldsymbol{i}}^{L}|| = ||\boldsymbol{k}_{\boldsymbol{o}}^{L}|| = ||\boldsymbol{k}_{\boldsymbol{i}}^{L} + \boldsymbol{g}_{\boldsymbol{hkl}}^{L}||. \tag{103}$$

$$||\boldsymbol{k}_{\boldsymbol{i}}^{L}|| = ||\boldsymbol{k}_{\boldsymbol{i}}^{L} + \underline{\boldsymbol{R}}^{L,S}\underline{\boldsymbol{R}}^{S,C}\boldsymbol{g}_{\boldsymbol{hkl}}^{C}||. \tag{104}$$

where we have defined $\underline{\boldsymbol{R}}^{S,C}$ as the crystal **orientation** and $\underline{\boldsymbol{R}}^{L,S}$ is completely defined by the rotation of the sample about a fixed axis $\hat{\boldsymbol{t}}$ by an angle ω (it could be multiple rotations, but the point is that we can build $\underline{\boldsymbol{R}}^{L,S}$ from experimental data). The figure below shows a typical example of the rotating crystal experiment.



1. Diffracting Crystal
2. Area Detector
3. Debye-Scherrer Ring

- Equations 103 and 104 are the fundamental equations of diffraction data reduction. The intercept of the diffracted beam with the detector is determined and from the geometry of the experiment and knowledge of the beam characteristics, $\boldsymbol{g}^L_{\boldsymbol{hkl}}$ can be computed for each diffraction spot produced by the crystal. We can think of the rotating crystal experiment in 2 ways. First, you can build use the concept of the rotating crystal experiment to build a **Virtual Diffractometer**[6] - for a given crystal orientation, experiment geometry and x-ray beam conditions, where will spots appear on the detector? So, at what angles (ω) will diffraction occur and what are the detector coordinates of the resulting spot? Building a Virtual Diffractometer is the first step towards understanding how the rotating crystal methods works. Everyone should do it.... We also use the Virtual Diffractometer extensively for interpretation of data and for comparison to models [7, 8, 9, 10]. There are many ways to solve for the ω angles that will produce diffraction. Here are some ideas.
  - Equation 104 is a scalar equation that can be solved to find the angle ω when diffraction events occur (or returning to Ewald's sphere construction, by what angle must we rotate the sample for $\boldsymbol{g_{hkl}}$ to contact the sphere). If $\hat{\boldsymbol{t}}$ is perpendicular to $\boldsymbol{k_i}$, Equation 104 has 0, 1 or 2 solutions.
    - ∗ We can rewrite equation Equation 104 as:

      $$F(\omega) = ||\boldsymbol{k}^L_{\boldsymbol{i}}|| - ||\boldsymbol{k}^L_{\boldsymbol{i}} + \underline{\boldsymbol{R}}^{L,S}(\omega)\underline{\boldsymbol{R}}^{S,C}\boldsymbol{g}^C_{\boldsymbol{hkl}}|| = 0 \tag{105}$$

      and find the roots of the equation (values of ω) numerically.
    - ∗ We can also recast the problem as a minimization problem:

      $$F(\omega) = \Big| ||\boldsymbol{k}^L_{\boldsymbol{i}}|| - ||\boldsymbol{k}^L_{\boldsymbol{i}} + \underline{\boldsymbol{R}}^{L,S}(\omega)\underline{\boldsymbol{R}}^{S,C}\boldsymbol{g}^C_{\boldsymbol{hkl}}|| \Big| \tag{106}$$

      and find the values of ω which minimize the function numerically (NOTE: the minima are equal to 0).
    - ∗ 32 Lastly, analytic solutions exist [1]
      - · If the beam is traveling in the $-\hat{\boldsymbol{e}}^L_{\boldsymbol{3}}$ direction and the rotation axis is $\hat{\boldsymbol{e}}^L_{\boldsymbol{2}}$

        $$||\boldsymbol{k}^L_{\boldsymbol{i}}||^2 = ||\boldsymbol{k}^L_{\boldsymbol{i}} + \underline{\boldsymbol{R}}^{L,S}(\omega)\underline{\boldsymbol{R}}^{S,C}\boldsymbol{g}^C_{\boldsymbol{hkl}}||^2$$

        $$(k^L_{i3})^2 = (k^L_{i3})^2 + ||\boldsymbol{g}||^2 + 2k^L_{i3}(\cos(\omega)g^S_3 - \sin(\omega)g^S_1)$$

        $$\cos(\omega)g^S_3 - \sin(\omega)g^S_1 = \frac{\lambda||\boldsymbol{g}||^2}{4\pi}$$
      - · If we define Y as

        $$Y = \frac{\lambda||\boldsymbol{g}||^2}{4\pi}$$

        $$\sqrt{1 - \sin^2(\omega)}g^S_3 = \sin(\omega)g^S_1 + Y$$

        $$(1 - \sin^2(\omega))(g^S_3)^2 = \sin^2(\omega)(g^S_1)^2 + 2\sin(\omega)g^S_1 Y + Y^2$$

        $$-\left((g^S_1)^2 + (g^S_3)^2\right)\sin^2(\omega) - 2g^S_1 Y\sin(\omega) + \left((g^S_3)^2 - Y^2\right) = 0$$

        $$A = -\left((g^S_1)^2 + (g^S_3)^2\right) \tag{107a}$$

$$B = -2 g_1^S Y \tag{107b}$$

$$C = (g_3^S)^2 - Y^2 \tag{107c}$$

· Finally:

$$\omega = \arcsin\left(\frac{-B \pm \sqrt{B^2 - 4AC}}{2A}\right) \tag{108}$$

∗ *NOTE: Equation 108 produces 4 solutions between $-180°$ and $180°$. Only two of these solutions satisfy Equation 104. After evaluating the analytic solution Equation 108, the two solutions which actually satisfy Equation 104 must be selected.

- From a data reduction perspective a set of diffraction spots and Equation 104 can be used to solve for the crystal orientation, $\underline{\boldsymbol{R}}^{S,C}$. There are many ways of doing this. Fable from the DTU group (appears on sorgeforge website and is referenced on the ESRF software site: http://www.esrf.eu/Instrumentation/software/data-analysis) is one software package, HEXRD from LLNL (https://e-reports-ext.llnl.gov/pdf/710553.pdf) is another. Again, for the beginner, there is nothing like writing your own version. In reality, we are interested in orientation and lattice strain both Fable and HEXRD can also determine lattice strain. We describe the set of equations to be solved for the current lattice orientation and strain state in a later section of this document.

5 Measuring Lattice Strain and Computing Crystal Stress

5.1 Overview

Diffraction forms the basis of a long list of important experiments. We will focus on a few specific diffraction-based tests/applications. Primarily, we use diffraction for:

1. determining the orientation (average) of a crystal
2. understanding the mechanical response of an individual crystal
   (a) Elastic response (average lattice strains)
   (b) Inelastic or elastic-plastic response (resolved shear stress on slip systems)
3. understanding the distributions of orientations and strains within a polycrystalline aggregate
   (a) creation of orientation pole figures
   (b) creation of strain pole figures
4. nondestructively constructing a grain (crystal) map from an aggregate
5. (**Note: the last 2 topics are not explicitly part of the NX school lecture**)

5.2 Motivation

This is where we start to blend material models and diffraction. There are a few important guiding principles:

1. crystal vs. aggregate, level of mechanical phenomenology, continuum point / representative volume element / material point:
   (a) a crystalline solid experiences anisotropic behavior on the single crystal scale but that changes when crystals are assembled into an aggregate,
   (b) concepts of stress, strain and deformation, in general, change from the crystal scale to the aggregate scale
2. concept of a diffraction volume and diffracted x-ray intensity distribution
   (a) One crystal - spots
   (b) Small polycrystal - spots
   (c) Larger polycrystal - rings
3. The elastic-plastic deformation of a crystalline solid produces some very distinct changes in the diffracted x-ray intensity

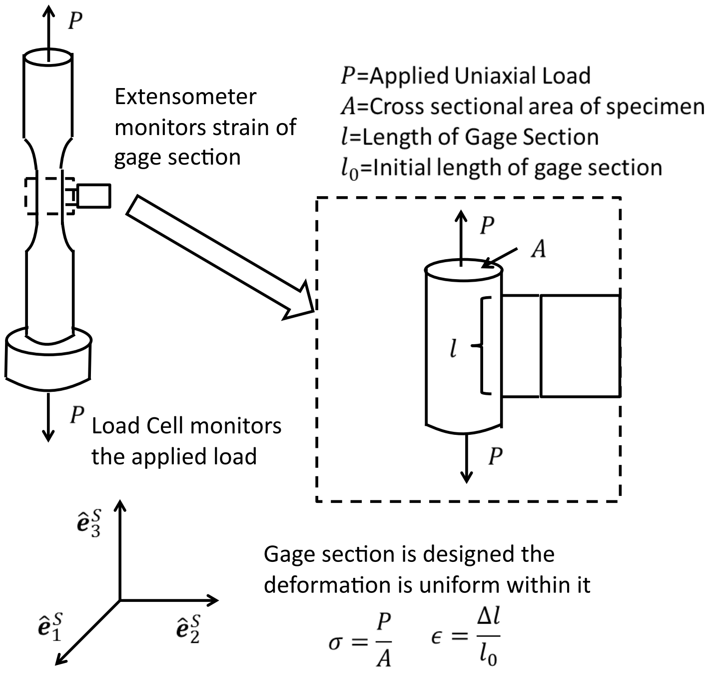
5.3 Approach

We (like many others) approach the use of diffraction data from a mechanics of materials / stress analysis perspective. The deformation of a crystal results in distortion, straining and rotation of the material. The crystal lattice is a fundamental quantity and we base much of our analysis on its straining and reorientation. We use some very basic engineering tools and analyses to understand crystal scale deformation.

1. The strain gage is one of the most fundamental sensors used by engineers. We use it to build other transducers such as load cells but we also use the strains themselves along with Hooke's law to understand the state of stress that an engineering component is experiencing. The crystal lattice can be viewed as "nature's strain gages" and we begin an understanding of our analysis of lattice strains on a classic method of reducing strain gage **rosette** data. This will give us the elastic state of strain within a crystal (tensor) and then we can compute the stress.
2. Armed with a knowledge of the stress being experienced by the crystal, we can begin to understand yielding (inelastic) behavior, which occurs due to a dislocation process known as crystallographic slip.
3. The rosette equations have some limitations on the extent of deformation. In a later section of this document, we will apply a full continuum mechanics analysis, that can used in a general way to not only understand the current state of strain being experienced by each crystal but its instantaneous lattice orientation.

5.4 Elastic-Plastic Behavior of Metallic Polycrystals

- Examine material behavior by looking at a uniaxial deformation sample

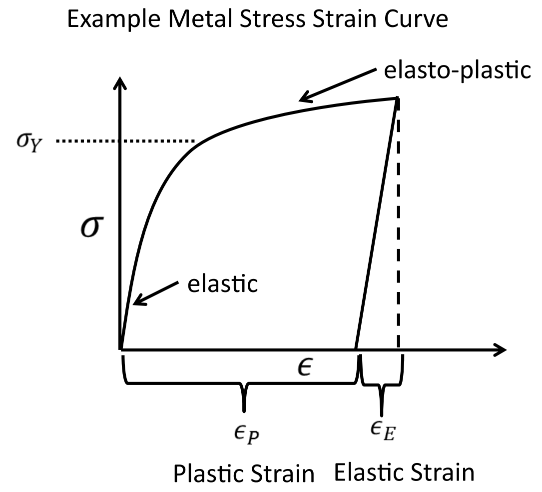


- The quantities σ and ϵ are actually components of the stress and strain tensors:

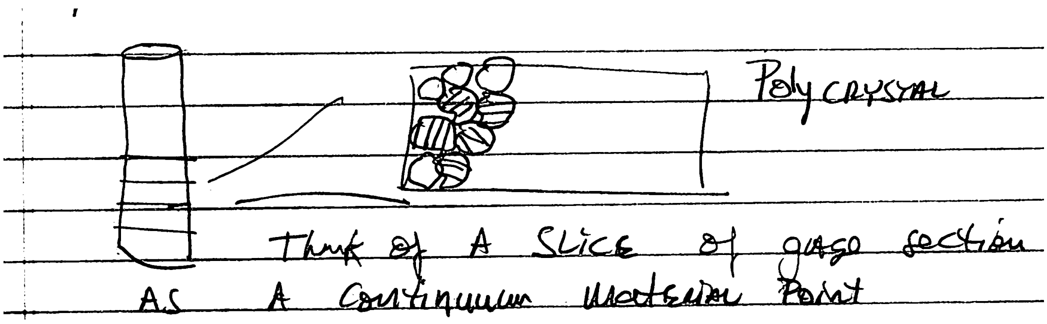
$$\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & P/A \end{bmatrix} \text{ and } \begin{bmatrix} -\nu\epsilon_{33} & 0 & 0 \\ 0 & -\nu\epsilon_{33} & 0 \\ 0 & 0 & \frac{\Delta l}{l_o} \end{bmatrix}$$

  respectively for isotropic elasticity. The main point is that the stress tensor contains one component. The strains ending up being whatever the material response is.

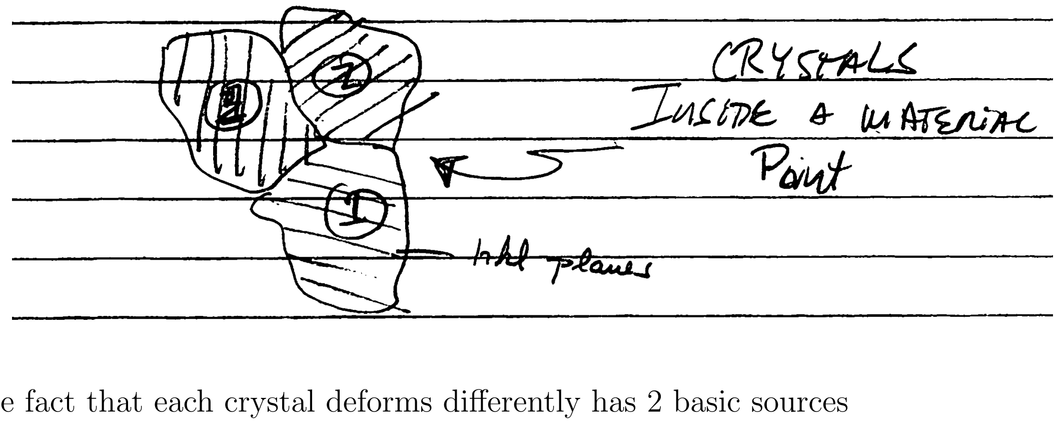
- A typical uniaxial stress-strain curve for a metal:



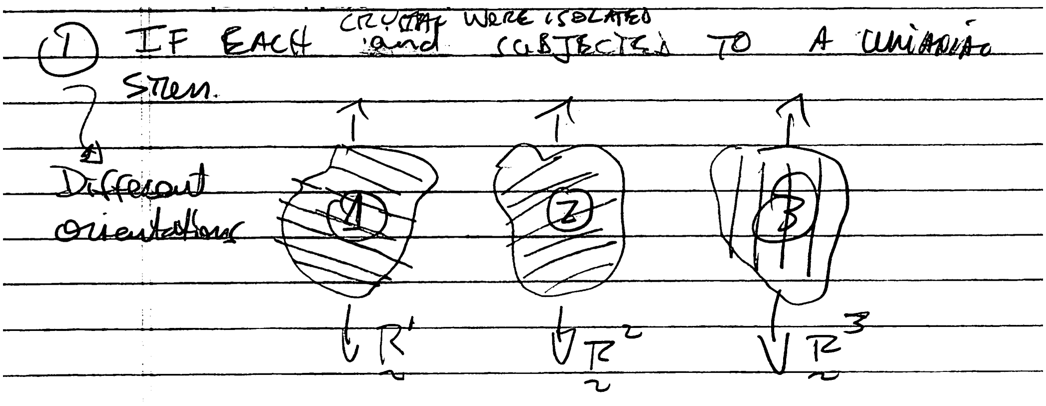
- The design of the sample assures that every "point" along the gage section experiences the same deformation

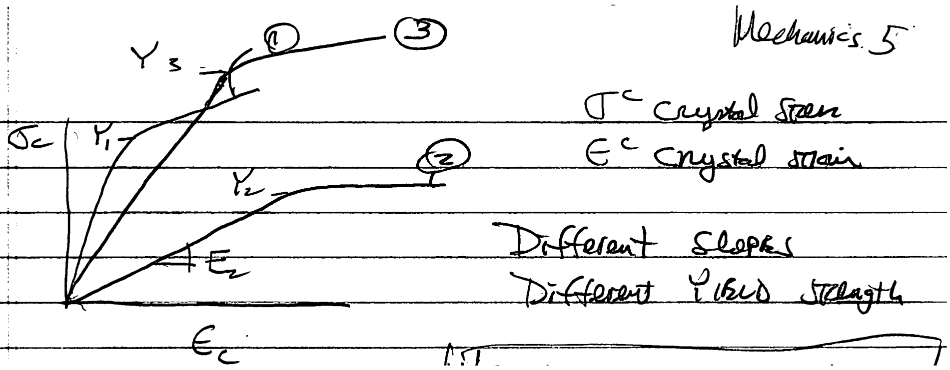


- The grain defines a natural phenomenological size scale - need "lots" of them to make up an aggregate. However, a material point could even be smaller than a grain. It all depends on what you are trying to model. Lets look at the behavior of individual grains within an aggregate:

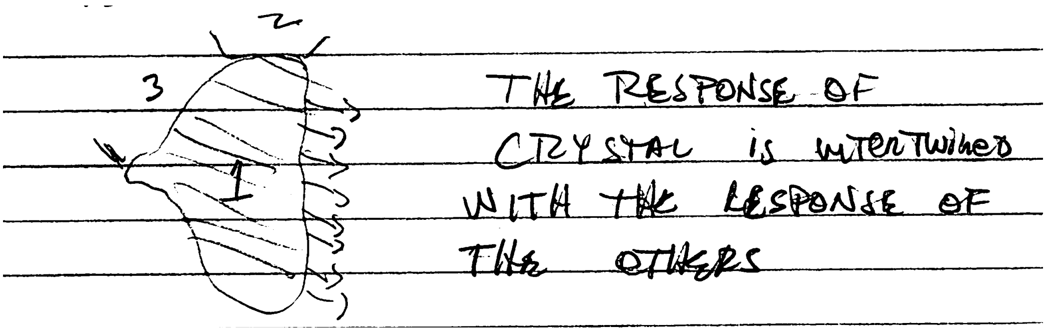


- The fact that each crystal deforms differently has 2 basic sources
  - The single crystal anisotropy - even if each crystal were subjected to uniaxial tension, the orientation of the crystal relative to the loading axis would dictate its behavior.



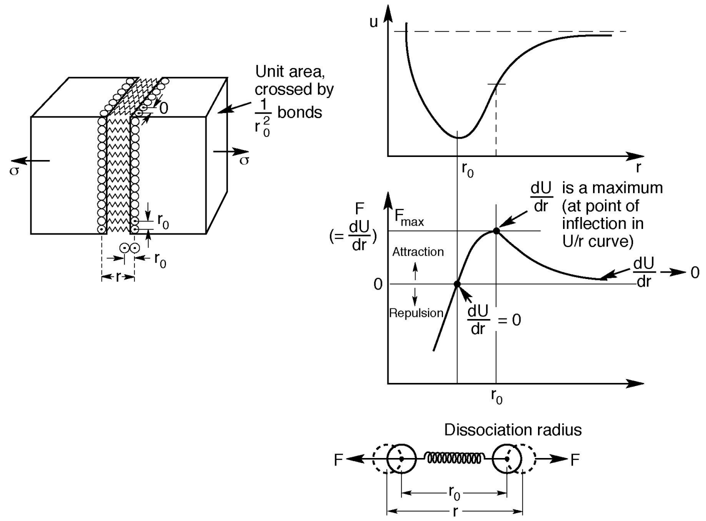


  - Each crystal is a structural unit being loaded by the structural units (crystals) next to it. The crystal stresses don't all have to be P/A, they only have to "add up" to P/A. That is, all of the axial load must be accounted for by the load carried by each crystal. We normalize that load by the total cross-sectional area in the definition of the uniaxial stress, P/A. Think of the aggregate as individual boundary value problems. In crystal plasticity this is often the hard part, linking the single crystal behavior to the polycrystal. These are issues related to mean field assumptions or linking hypotheses.



5.5 Physical sources of Elastic and Plastic Deformation Behavior

- Elastic deformation at the crystal scale can be envisioned with linear springs replacing the atomic bonds. The equilibrium position (r_o) is the point where the potential energy, U, is minimized. As the bond is stretched or compressed, U increases and when the load is removed, the system goes back to equilibrium. Like a linear spring, the force, F, can be determined by differentiating the U(r) curve.

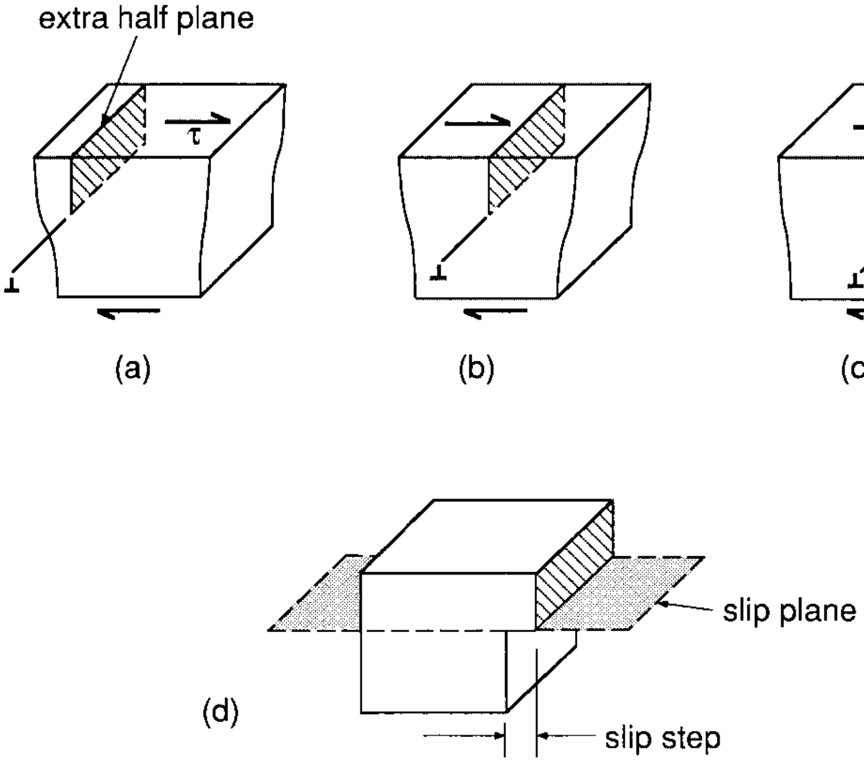


- So, elastic strains stretch atomic bonds and change d spacing. In a diffraction experiment, incoming x-rays ($\boldsymbol{k_i}$) are diffracted and we determine the outgoing x-ray beam ($\boldsymbol{k_o}$) from the spot on the detector. We can calculate the scattering vector as $\boldsymbol{q} = \boldsymbol{k_o} - \boldsymbol{k_i}$ and we know that diffraction only happens when Laue condition is satisfied, $\boldsymbol{q} = \boldsymbol{g_{hkl}}$. From $\boldsymbol{g_{hkl}}$ we determine the lattice spacing, $d_{hkl} = \frac{2\pi}{||\boldsymbol{g_{hkl}}||}$ and the orientation of the associated planes, $\boldsymbol{n_{hkl}} = \frac{\boldsymbol{g_{hkl}}}{||\boldsymbol{g_{hkl}}||}$ (we've dropped the hat). So, the **lattice strain** in the direction of $\boldsymbol{n_{hkl}}$ is

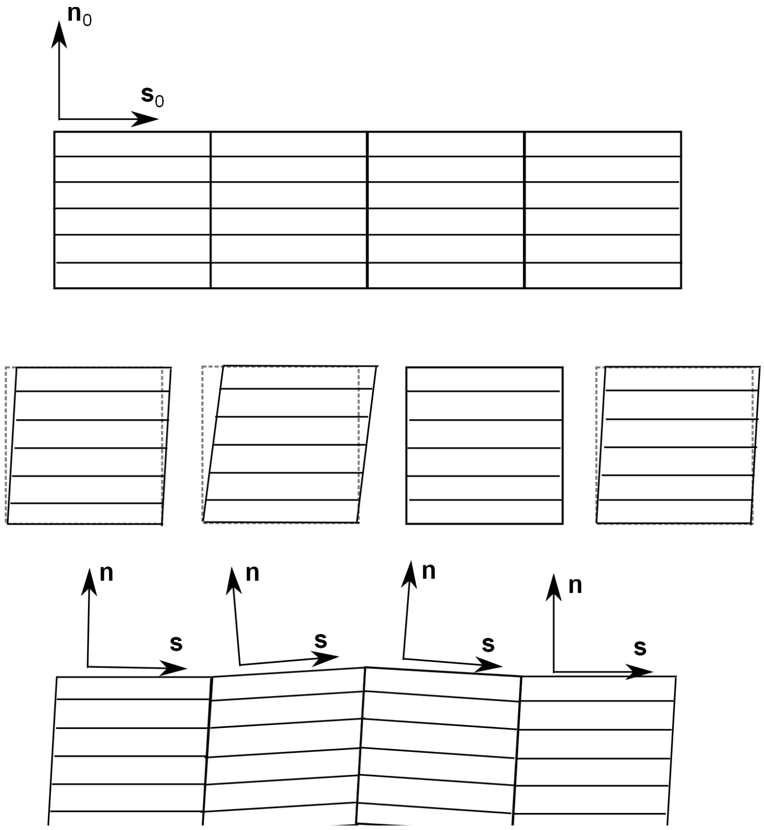
$$\epsilon_{nn} = \frac{\Delta d_{hkl}}{d^o_{hkl}} = \frac{d_{hkl} - d^o_{hkl}}{d^o_{hkl}} = \frac{d_{hkl}}{d^o_{hkl}} - 1 = \frac{||\boldsymbol{g^o_{hkl}}||}{||\boldsymbol{g_{hkl}}||} - 1 \tag{109}$$

  where d^o_{hkl} and $\boldsymbol{g^o_{hkl}}$ are the unstrained lattice spacing and reciprocal lattice vector, respectively. With enough lattice strain measurements, we can "build" the lattice (elastic) strain tensor and calculate stress!!!!! We will develop this.

- Plastic deformation is about the creation and movement of defects in the crystal lattice through the crystal. The most common is the line defect known as a dislocation. An edge dislocation (shown below) is an extra half plane of atoms. As can be seen, under the application of a shear stress, a dislocation can pass entirely through a perfect crystal and leave the lattice unchanged. The only evidence that the dislocation passed through the crystal is the step that is produced at the crystal boundary.



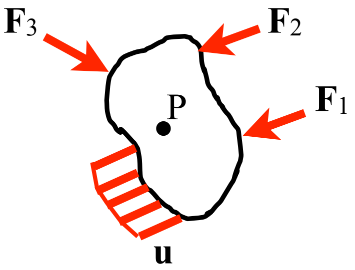
- The figure above is completely idealized. Plasticity isn't about the motion of a single dislocation. In a real crystal, a set of dislocations move through the lattice at different rates - some "sticking" more than others. The result is the creation of "wrinkles" or curvature in the lattice. This is shown below. The effect on the diffraction signal is that one lattice plane normal has become several. The associated $\boldsymbol{g_{hkl}}$'s will now pick slightly different scattering vectors ($\boldsymbol{q}$'s) and the diffracted intensity "spot" on the detector will spread. This spread is an indicator of plasticity-induced heterogeneity. We'll talk more about this later.



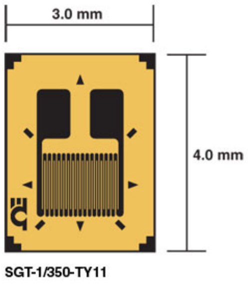
5.6 Reducing Strain Gage Data

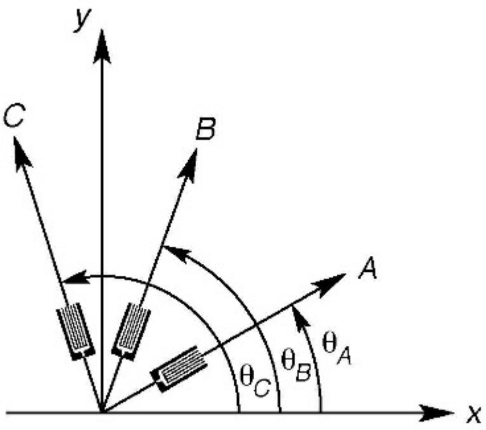
- The simplest way to think about reducing lattice strain data from a crystal is by thinking of the lattice planes as tiny little strain gages. The normal strains defined above look just like the normal strains that we measure using engineering strain gages. We develop here, the standard equations for reducing strain gage data. We will then apply this analysis to the problem of lattice strains. There are many good references for strain gages and strain data reduction. Here is one of the best [11].

- Consider a body (macroscopic) being loaded by forces or displacements as shown below. Engineering stress analysis is a method of using linear strain gages and Hooke's law to determine the state of stress somewhere on the surface of the loaded body.



- Resistance strain gages turn the change in the resistance measured within the length of the wire in the gage into a strain. Several gages can be arranged into a strain gage rosette to measure normal strains in multiple directions.





- The state of plane stress on the surface of an elastically isotropic component produces the following stress and strain tensors relative to x,y,z:

$$\begin{bmatrix} \sigma_{11} & \sigma_{12} & 0 \\ \sigma_{12} & \sigma_{22} & 0 \\ 0 & 0 & 0 \end{bmatrix} \text{ and } \begin{bmatrix} \epsilon_{11} & \epsilon_{12} & 0 \\ \epsilon_{21} & \epsilon_{22} & 0 \\ 0 & 0 & \epsilon_{33} \end{bmatrix}$$

  So the business of experimental stress analysis is to take the normal strains from a rosette and determine the strain tensor. Note that the plane stress conditions will enable the determination of the out of plane normal stress, ϵ_{33}, once we know the in-plane components so we need 3 normal strains to fix the strain tensor.

- We'll look at 2 methods of determining $[\epsilon]$. First we will think of transforming the strain tensor from x,y,z to the local coordinate system associated with each of the strain gages. Recall the transformation equations for a second order tensor from an old to a new (primed) coordinate system: $\epsilon'_{ij} = \epsilon_{kl} a_{ik} a_{jl}$, where $a_{ij} = \hat{\boldsymbol{e}}'_i \cdot \hat{\boldsymbol{e}}_j$. In this case, the coordinate transformation is a simple rotation around z by θ_A, θ_B or θ_C and the prime basis vectors are:

$$\hat{\boldsymbol{e}}'_1 = cos(\theta_I)\hat{\boldsymbol{e}}_1 + sin(\theta_I)\hat{\boldsymbol{e}}_2 \tag{110}$$

$$\hat{\boldsymbol{e}}'_2 = -sin(\theta_I)\hat{\boldsymbol{e}}_1 + cos(\theta_I)\hat{\boldsymbol{e}}_2 \tag{111}$$

  and

$$[a] = \begin{bmatrix} \cos(\theta_I) & \sin(\theta_I) & 0 \\ -\sin(\theta_I) & \cos(\theta_I) & 0 \\ 0 & 0 & 1 \end{bmatrix} \tag{112}$$

  just like the simple rotation matrices we defined earlier. So now

$$[\epsilon]' = [a][\epsilon][a]^T \tag{113}$$

$$= \begin{bmatrix} c & s & 0 \\ -s & c & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} \epsilon_{11} & \epsilon_{12} & 0 \\ \epsilon_{21} & \epsilon_{22} & 0 \\ 0 & 0 & \epsilon_{33} \end{bmatrix} \begin{bmatrix} c & -s & 0 \\ s & c & 0 \\ 0 & 0 & 1 \end{bmatrix} \tag{114}$$

$$= \begin{bmatrix} c & s & 0 \\ -s & c & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} \epsilon_{11}c + \epsilon_{12}s & -\epsilon_{11}s + \epsilon_{12}c & 0 \\ -\epsilon_{12}c + \epsilon_{22}s & -\epsilon_{12}s + \epsilon_{22}c & 0 \\ 0 & 0 & \epsilon_{33} \end{bmatrix} \tag{115}$$

$$= \begin{bmatrix} \epsilon_{11}c^2 + 2\epsilon_{12}sc + \epsilon_{22}s^2 & -- & -- \\ -- & -- & -- \\ -- & -- & -- \end{bmatrix} \tag{116}$$

All we need is the ϵ'_{11} term so we can repeat the process for each gage angle and write the following system of equations relating the strains measured at the three orientations, ϵ_A, ϵ_B, ϵ_C to the strain tensor, $\underline{\boldsymbol{\epsilon}}$ as

$$\epsilon_A(\theta_A) = cos^2(\theta_A)\epsilon_{11} + sin^2(\theta_A)\epsilon_{22} + 2sin(\theta_A)cos(\theta_A)\epsilon_{12} \tag{117}$$
$$\epsilon_B(\theta_B) = cos^2(\theta_B)\epsilon_{11} + sin^2(\theta_B)\epsilon_{22} + 2sin(\theta_B)cos(\theta_B)\epsilon_{12} \tag{118}$$
$$\epsilon_C(\theta_C) = cos^2(\theta_C)\epsilon_{11} + sin^2(\theta_C)\epsilon_{22} + 2sin(\theta_C)cos(\theta_C)\epsilon_{12} \tag{119}$$

We call these the rosette equations and we solve them simultaneously for ϵ_{11}, ϵ_{12} and ϵ_{22}.

- If we make more than 3 strain measurements, this becomes a least squares problem. Using $\sigma_{33} = 0$, we get
$$\epsilon_{33} = \frac{-\nu}{1-\nu}(\epsilon_{11} + \epsilon_{22}) \tag{120}$$
- With $\boldsymbol{\epsilon}$, we can use Hooke's law to calculate the stress tensor, $\boldsymbol{\sigma}$.
- Care must be taken so that θ_A, θ_B and θ_C effectively span the directions necessary to effectively quantify $\boldsymbol{\epsilon}$. There are ways to choose the angles to make the calculations easy, i.e. $\theta_A = 0$, $\theta_B = 45^o$, $\theta_C = 90^o$.
- Another way of generating the rosette equation is to use the nonion form of the strain tensor and take dot products to "pick out" a single component. We do this all the time with vectors, $\mathbf{v} = v_i\mathbf{\hat{e}_i}$, we pick out the component of $\mathbf{v}$ in a particular direction, $\mathbf{\hat{n}}$, with a dot product,
$$\begin{aligned} v_n &= \mathbf{v} \cdot \mathbf{\hat{n}} \\ &= v_i\hat{\boldsymbol{e}}_i \cdot n_j\hat{\boldsymbol{e}}_j \\ &= v_i n_j(\hat{\boldsymbol{e}}_i \cdot \hat{\boldsymbol{e}}_j) \\ &= v_i n_j \delta_{ij} \end{aligned}$$
- The beauty of the full nonion form is the intuitive way for choosing a particular component of a second order tensor comes out by doing 2 dot products (for each index). Recall the notion form:
$$\begin{aligned} \underline{\boldsymbol{\epsilon}} = \epsilon_{ij}\mathbf{\hat{e}_i\hat{e}_j} = \epsilon_{11}\mathbf{\hat{e}_1\hat{e}_1} + \epsilon_{12}\mathbf{\hat{e}_1\hat{e}_2} + \epsilon_{13}\mathbf{\hat{e}_1\hat{e}_3} + \\ \epsilon_{21}\mathbf{\hat{e}_2\hat{e}_1} + \epsilon_{22}\mathbf{\hat{e}_2\hat{e}_2} + \epsilon_{23}\mathbf{\hat{e}_2\hat{e}_3} \\ +\epsilon_{31}\mathbf{\hat{e}_3\hat{e}_1} + \epsilon_{32}\mathbf{\hat{e}_3\hat{e}_2} + \epsilon_{33}\mathbf{\hat{e}_3\hat{e}_3} \end{aligned}$$

Now, determine ϵ_{nn} by dotting each of the basis vectors, i.e.

$$\epsilon_{nn} = (\epsilon_{ij}\hat{\boldsymbol{e}}_i\hat{\boldsymbol{e}}_j) \cdot (n_k\hat{\boldsymbol{e}}_k) \cdot (n_l\hat{\boldsymbol{e}}_l)$$
$$\epsilon_{nn} = \epsilon_{ij}n_k(\hat{\boldsymbol{e}}_i \cdot \hat{\boldsymbol{e}}_k)n_l(\hat{\boldsymbol{e}}_j \cdot \hat{\boldsymbol{e}}_l)$$
$$\epsilon_{nn} = \epsilon_{ij}n_k n_l \delta_{ik}\delta_{jl}$$
$$\epsilon_{nn} = \epsilon_{ij}n_i n_j \tag{121}$$

or

$$\epsilon_{nn} = \mathbf{\hat{n}} \cdot \underline{\boldsymbol{\epsilon}} \cdot \mathbf{\hat{n}} \tag{122}$$

- So, in our case for the gage aligned with θ_A, $\hat{\mathbf{n}} = cos(\theta_A)\hat{\boldsymbol{e}}_1 + sin(\theta_A)\hat{\boldsymbol{e}}_2$ and

$$\epsilon_{nn} = \epsilon_A = \begin{bmatrix} cos(\theta_A) & sin(\theta_A) & 0 \end{bmatrix} \begin{bmatrix} \epsilon_{11} & \epsilon_{12} & 0 \\ \epsilon_{21} & \epsilon_{22} & 0 \\ 0 & 0 & \epsilon_{33} \end{bmatrix} \begin{bmatrix} cos(\theta_A) \\ sin(\theta_A) \\ 0 \end{bmatrix} \tag{123}$$

$$\epsilon_{nn} = \epsilon_A = cos^2(\theta_A)\epsilon_{11} + sin^2(\theta_A)\epsilon_{22} + 2sin(\theta_A)cos(\theta_A)\epsilon_{12}$$

  With similar equations for θ_B and θ_C, same as above. This works with any second order tensor.

- If we have multiple lattice strain measurements ($\epsilon_n n, i$ where the index i indicates a specific measurement), we can express Equation 121 conveniently in matrix form.

- We see that if Equation 121 is fully written out:

$$\epsilon_{nn} = n_1^2\epsilon_{11} + n_2^2\epsilon_{22} + n_3^2\epsilon_{33} + 2n_2n_3\epsilon_{23} + 2n_1n_3\epsilon_{13} + 2n_1n_2\epsilon_{12} \tag{124}$$

- Using this form we can construct a matrix $\boldsymbol{N}$ which will enable us to express the set of lattice strain measurements as a linear system of equations:

$$\begin{bmatrix} \epsilon_{nn,1} \\ \epsilon_{nn,2} \\ \cdots \end{bmatrix} = \begin{bmatrix} n_{1,1}^2 & n_{2,1}^2 & n_{3,1}^2 & n_{2,1}n_{3,1} & n_{1,1}n_{3,1} & n_{1,1}n_{2,1} \\ n_{1,2}^2 & n_{2,2}^2 & n_{3,2}^2 & n_{2,2}n_{3,2} & n_{1,2}n_{3,2} & n_{1,2}n_{2,2} \\ \cdots & & & & & \end{bmatrix} \begin{bmatrix} \epsilon_{11} \\ \epsilon_{22} \\ \epsilon_{33} \\ 2\epsilon_{23} \\ 2\epsilon_{13} \\ 2\epsilon_{12} \end{bmatrix} \tag{125}$$

- With this form, we can see that if we have 6 lattice strain measurements, we can invert $\boldsymbol{N}$ to find the lattice strain tensor ($\underline{\boldsymbol{\epsilon}}$) components. With more than 6 measurements, a least squares process can be used to find $\underline{\boldsymbol{\epsilon}}$.

5.7 Determining the Crystal Strains from Diffraction Data

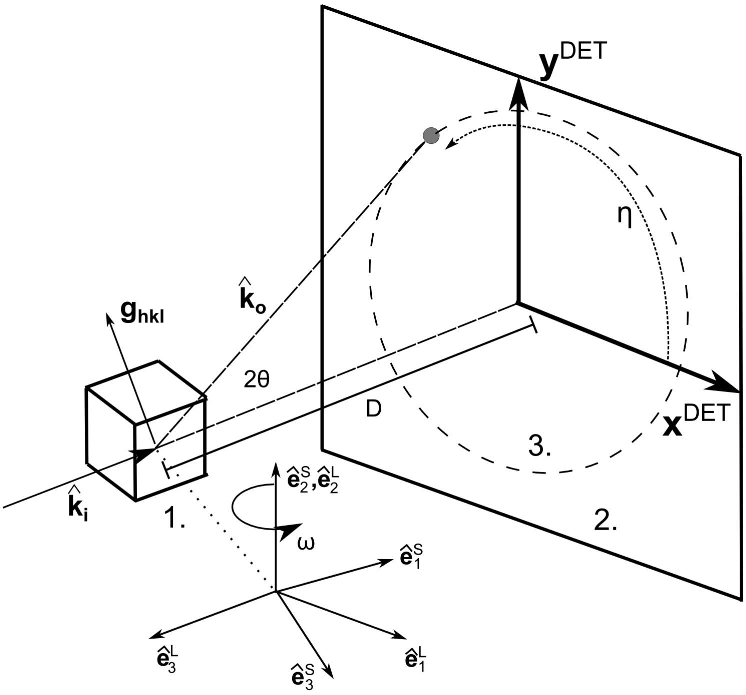
- We will basically repeat the rosette process for the determination of the state of strain within a crystal using measured lattice strains from a rotating crystal experiment and $\epsilon_{nn} = \hat{\mathbf{n}} \cdot \underline{\boldsymbol{\epsilon}} \cdot \hat{\mathbf{n}}$.

- The rotating crystal experiment is shown schematically below. Every diffraction spot can be associated with the triplet of relevant angles from the experiment $(\eta, 2\theta, \omega)$. The angle ω comes from the diffractometer and we measure η and 2θ from the intersection point of the diffracted beam on the detector.

- As discussed previously we want to measure $\boldsymbol{g_{hkl}}$ because the reading from the "strain gage" can be determined, $\epsilon_{nn} = \frac{\Delta d_{hkl}}{d_{hkl}^o} = \frac{||\boldsymbol{g_{hkl}^o}||}{||\boldsymbol{g_{hkl}}||} - 1$ and the orientation of the "strain gage" is given by $\boldsymbol{n_{hkl}} = \frac{\boldsymbol{g_{hkl}}}{||\boldsymbol{g_{hkl}}||}$.

- We use the definition of the scattering vector and the Laue condition, $\boldsymbol{q} = \boldsymbol{k_o} - \boldsymbol{k_i} = \boldsymbol{g_{hkl}}$ to understand that if we can determine $\boldsymbol{k_o}$ and $\boldsymbol{k_i}$ we can compute $\boldsymbol{g_{hkl}}$.

- The x-ray beam is usually fixed during an experiment with respect to the laboratory coordinate systems. Due to this it will be more convenient to work with components of vectors in the laboratory coordinate systems (the scripts indicate components of vector,



1. Diffracting Crystal
2. Area Detector
3. Debye-Scherrer Ring

remembering that the vector is comprised of the component values multiplied by the basis vectors), so that

$$\boldsymbol{g}^L_{\boldsymbol{hkl}} = \boldsymbol{k}^L_{\boldsymbol{o}} - \boldsymbol{k}^L_{\boldsymbol{i}}$$

and since $\boldsymbol{g}_{\boldsymbol{hkl}}$ is more easily defined relative to the crystal basis

$$\underline{\boldsymbol{R}}^{L,S}\underline{\boldsymbol{R}}^{S,C}\boldsymbol{g}^C_{\boldsymbol{hkl}} = \boldsymbol{k}^L_{\boldsymbol{o}} - \boldsymbol{k}^L_{\boldsymbol{i}}$$

- So we set up the lab frame around the incoming beam,

$$\boldsymbol{k}^L_{\boldsymbol{i}} = -\frac{2\pi}{\lambda}\begin{bmatrix}0\\0\\1\end{bmatrix}$$

- Now, we determine $\boldsymbol{k}^L_{\boldsymbol{o}}$ from the geometry of the experiment. There are probably lots of ways to do this. One way is to just to get the unit vector, $\hat{\boldsymbol{k}}_{\boldsymbol{o}}$ from the position vector from the sample to the spot on the detector (call this $\boldsymbol{k}^*_{\boldsymbol{o}}$) and you know that the magnitude of $\boldsymbol{k}_{\boldsymbol{o}}$ is $2\pi/\lambda$ the same as $\boldsymbol{k}_{\boldsymbol{i}}$.

- So $\boldsymbol{k}^*_{\boldsymbol{o}} = k^{*1}_o\hat{\mathbf{e}}^{\mathbf{L}}_{\mathbf{1}} + k^{*2}_o\hat{\mathbf{e}}^{\mathbf{L}}_{\mathbf{2}} + k^{*3}_o\hat{\mathbf{e}}^{\mathbf{L}}_{\mathbf{3}}$. Clearly $k^{*3}_o = -D$. The 1 and 2 components of $\boldsymbol{k}^*_{\boldsymbol{o}}$ are just the coordinates of the intercept of the diffracted beam on the detector $\boldsymbol{\xi}$. We would like to put those into terms of the angles η and θ. The radius of the Debye ring is $\mathrm{D}\tan 2\theta$ so

$$\xi_1 = D\tan 2\theta\cos\eta \quad \text{and} \quad \xi_2 = D\tan 2\theta\sin\eta$$

So

$$\boldsymbol{k}^*_{\boldsymbol{o}} = (D\tan 2\theta\cos\eta)\hat{\mathbf{e}}^{\mathbf{L}}_{\mathbf{1}} + (D\tan 2\theta\sin\eta)\hat{\mathbf{e}}^{\mathbf{L}}_{\mathbf{2}} - D\hat{\mathbf{e}}^{\mathbf{L}}_{\mathbf{3}} \tag{126}$$

- We can now determine

$$\begin{aligned}\hat{\boldsymbol{k}}_{\boldsymbol{o}} = \frac{\boldsymbol{k}_{\boldsymbol{o}}^*}{||\boldsymbol{k}_{\boldsymbol{o}}^*||} &= \frac{\boldsymbol{k}_{\boldsymbol{o}}^*}{\sqrt{D^2\tan^2 2\theta\cos^2\eta + D^2\tan^2 2\theta\sin^2\eta + D^2}} \\ &= \frac{\boldsymbol{k}_{\boldsymbol{o}}^*}{D\sqrt{\tan^2 2\theta + 1}} = \frac{\boldsymbol{k}_{\boldsymbol{o}}^*\cos 2\theta}{D} \\ \hat{\boldsymbol{k}}_{\boldsymbol{o}} &= (\sin 2\theta\cos\eta)\mathbf{\hat{e}_1^L} + (\sin 2\theta\sin\eta)\mathbf{\hat{e}_2^L} - \cos 2\theta\mathbf{\hat{e}_3^L} \end{aligned} \tag{127}$$

- So

$$\boldsymbol{k}_{\boldsymbol{o}}^L = \frac{2\pi}{\lambda}\hat{\boldsymbol{k}}_{\boldsymbol{o}}^L = \frac{2\pi}{\lambda}\begin{bmatrix}\sin 2\theta\cos\eta \\ \sin 2\theta\sin\eta \\ -\cos 2\theta\end{bmatrix} \tag{128}$$

- Now

$$\begin{aligned}\boldsymbol{g}_{\boldsymbol{hkl}}^L = \boldsymbol{k}_{\boldsymbol{o}}^L - \boldsymbol{k}_{\boldsymbol{i}}^L &= \frac{2\pi}{\lambda}\begin{bmatrix}\sin 2\theta\cos\eta \\ \sin 2\theta\sin\eta \\ -\cos 2\theta + 1\end{bmatrix} \\ &= \frac{2\pi}{\lambda}\begin{bmatrix}2\sin\theta\cos\theta\cos\eta \\ 2\sin\theta\cos\theta\sin\eta \\ 2\sin^2\theta\end{bmatrix} = \frac{4\pi\sin\theta}{\lambda}\begin{bmatrix}\cos\theta\cos\eta \\ \cos\theta\sin\eta \\ \sin\theta\end{bmatrix}\end{aligned} \tag{129}$$

- We want the strains in the sample coordinates, so we transform,

$$\boldsymbol{g}_{\boldsymbol{hkl}}^S = \underline{\boldsymbol{R}}^{S,L}\boldsymbol{g}_{\boldsymbol{hkl}}^L \tag{130}$$

- Now we will have a list of lattice strains that we can apply the system of rosette equations to. Just like the strain gage rosette, we make many measurements. If we make more than 6, we can use least squares for the tensor.

- We derived this from the spots measured for one crystal, but you could also have many spots from many crystals. If you could identify the spots from each crystal, you can determine the strain tensor for each of them. You could also determine the list of lattice strains from a powder pattern (integrate azimuthally and create a "spot"). The interpretation of these lattice strains are a more advanced topic - we'll talk about it soon.

- How consistent is the rosette approach in terms of continuum mechanics? The strain gage stretches and rotates. Using the rosette equations, we don't take the rotation into account. As long as a small strain assumption is still valid, the rosette approach is OK. We will show a more exact approach later.

- We have the same concerns with diffraction. We determine $\boldsymbol{g}_{\boldsymbol{hkl}}$ before and after loading and the direction changes (just like the gage rotating). We choose one direction and determine the change in the g-vector length. Again, as long as the strains are "small", everything is OK. However, it is the rotation of the lattice associated with the plastic straining process that can create the bigger problems. If you become worried about that, there is a more sophisticated mechanistically-consistent method that we will develop later.

5.8 Crystal Elasticity - Computing Stress from Lattice Strains

- Now, knowing the strain tensor that the crystal is experiencing, we can calculate the crystal stress using Hooke's Law:

$$\sigma_{ij} = C_{ijkl}\epsilon_{kl}\text{or}\epsilon_{ij} = S_{ijkl}\sigma_{kl}$$

- The graduate solid mechanics course that you took spent a lot of time on this, so we will only develop the parts that are most closely related to diffraction. Here are some good references: [12, 13, 14]. We begin by introducing simplified (reduced) notation: $\sigma_i = C_{ij}\epsilon_j$ or $\epsilon_i = S_{ij}\sigma_j$. Where C_{ij} and S_{ij} are the stiffness and compliance matrices (not tensors) with

  $\sigma_1 = \sigma_{11} \quad \epsilon_1 = \epsilon_{11}$
  $\sigma_2 = \sigma_{22} \quad \epsilon_2 = \epsilon_{22}$
  $\sigma_3 = \sigma_{33} \quad \epsilon_3 = \epsilon_{33}$
  $\sigma_4 = \sigma_{23} \quad \epsilon_4 = 2\epsilon_{23}$
  $\sigma_5 = \sigma_{13} \quad \epsilon_5 = 2\epsilon_{13}$
  $\sigma_6 = \sigma_{12} \quad \epsilon_6 = 2\epsilon_{12}$

  Now we have 21 constants since [C] is symmetric. Also $[S] = [C]^{-1}$.

- As we start to introduce material symmetries, the number of non-zero constants gets smaller. There are many ways to derive the number of constants for a particular symmetry group. Herekovitch [12] and Ting [13] are pretty good. The results are below.

- These constants could be used directly if the sample and crystal coordinate systems coincided. What happens if they don't? We could transform the strain tensor from the sample to the crystal, use the canonical values of the stiffness to get the stress, then transform it back to the sample. We could also transform the elastic constants. To do that, we could re-convert [C] and [S] into fourth order tensors and transform to the prime system $C'_{ijkl} = a_{im}a_{jn}a_{ko}a_{lp}C_{mnop}$ and $S'_{ijkl} = a_{im}a_{jn}a_{ko}a_{lp}S_{mnop}$, where $a_{ij} = \hat{\boldsymbol{e}}'_i \cdot \hat{\boldsymbol{e}}_j$. Instead, we could derive rules for transforming the [C] and [S] matrices and the $\{\sigma\}$ and $\{\epsilon\}$ vectors. Here are the rules (from Ting)

$$\{\sigma\}' = [K]\{\sigma\}' \quad \text{and} \quad \{\epsilon\}' = \left([K]^{-1}\right)^T \{\epsilon\}' \tag{131}$$

and

$$[C]' = [K][C][K]^T \quad \text{and} \quad [S]' = \left([K]^{-1}\right)^T [S][K]^{-1} \tag{132}$$

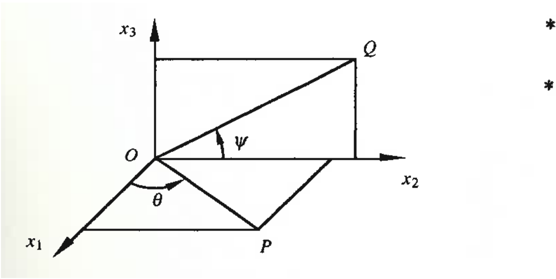
where

$$[K] = \begin{bmatrix} [K]_1 & 2[K]_2 \\ [K]_3 & [K]_4 \end{bmatrix} \quad \text{and} \quad [K]_1 = \begin{bmatrix} a_{11}^2 & a_{12}^2 & a_{13}^2 \\ a_{21}^2 & a_{22}^2 & a_{23}^2 \\ a_{31}^2 & a_{32}^2 & a_{33}^2 \end{bmatrix}$$

$$[K]_2 = \begin{bmatrix} a_{12}a_{13} & a_{13}a_{11} & a_{11}a_{12} \\ a_{22}a_{23} & a_{23}a_{21} & a_{21}a_{22} \\ a_{32}a_{33} & a_{33}a_{31} & a_{31}a_{32} \end{bmatrix}$$

$$[K]_3 = \begin{bmatrix} a_{21}a_{31} & a_{22}a_{32} & a_{23}a_{33} \\ a_{31}a_{11} & a_{32}a_{12} & a_{33}a_{13} \\ a_{11}a_{21} & a_{12}a_{22} & a_{13}a_{23} \end{bmatrix}$$

$$[K]_4 = \begin{bmatrix} a_{22}a_{33} + a_{23}a_{32} & a_{23}a_{31} + a_{21}a_{33} & a_{21}a_{32} + a_{22}a_{31} \\ a_{32}a_{13} + a_{33}a_{12} & a_{33}a_{11} + a_{31}a_{13} & a_{31}a_{12} + a_{32}a_{11} \\ a_{12}a_{23} + a_{13}a_{22} & a_{13}a_{21} + a_{11}a_{23} & a_{11}a_{22} + a_{12}a_{21} \end{bmatrix}$$



$\ast$	indicates a possibly nonzero element
$\ast$—$\ast$	indicates the two elements are equal
$\ast$—$\bar{\ast}$	indicates the two elements are equal but opposite in signs
$\otimes$	indicates $C_{66}=\frac{1}{2}(C_{11}-C_{12})$
m	indicates the number of independent elastic constants

(I) **Triclinic Materials.** No symmetry planes exist.

$$\mathbf{C}=\begin{bmatrix} \ast & \ast & \ast & \ast & \ast & \ast \\ & \ast & \ast & \ast & \ast & \ast \\ & & \ast & \ast & \ast & \ast \\ & & & \ast & \ast & \ast \\ & & & & \ast & \ast \\ & & & & & \ast \end{bmatrix}, \quad m=21.$$

(II) **Monoclinic Materials.** One symmetry plane.

(a) Symmetry plane at $x_1=0$, i.e., $\theta=0$.

$$\mathbf{C}=\begin{bmatrix} \ast & \ast & \ast & \ast & 0 & 0 \\ & \ast & \ast & \ast & 0 & 0 \\ & & \ast & \ast & 0 & 0 \\ & & & \ast & 0 & 0 \\ & & & & \ast & \ast \\ & & & & & \ast \end{bmatrix}, \quad m=13.$$

(b) Symmetry plane at $x_2=0$, i.e., $\theta=\pi/2$ or $\psi=0$.

$$\mathbf{C}=\begin{bmatrix} \ast & \ast & \ast & 0 & \ast & 0 \\ & \ast & \ast & 0 & \ast & 0 \\ & & \ast & 0 & \ast & 0 \\ & & & \ast & 0 & \ast \\ & & & & \ast & 0 \\ & & & & & \ast \end{bmatrix}, \quad m=13.$$

(c) Symmetry plane at $x_3=0$, i.e., $\psi=\pi/2$.

$$\mathbf{C}=\begin{bmatrix} \ast & \ast & \ast & 0 & 0 & \ast \\ & \ast & \ast & 0 & 0 & \ast \\ & & \ast & 0 & 0 & \ast \\ & & & \ast & \ast & 0 \\ & & & & \ast & 0 \\ & & & & & \ast \end{bmatrix}, \quad m=13.$$

(III) **Orthotropic (or Rhombic) Materials.** The three coordinate planes $\theta=0$, $\pi/2$, and $\psi=\pi/2$ are the symmetry planes.

$$\mathbf{C}=\begin{bmatrix} \ast & \ast & \ast & 0 & 0 & 0 \\ & \ast & \ast & 0 & 0 & 0 \\ & & \ast & 0 & 0 & 0 \\ & & & \ast & 0 & 0 \\ & & & & \ast & 0 \\ & & & & & \ast \end{bmatrix}, \quad m=9. \qquad (2.6\text{-}4)$$

(IV) **Trigonal Materials.** Three symmetry planes at $\theta=0$ and $\pm\pi/3$.

$$\mathbf{C}=\begin{bmatrix} \ast & \ast & \ast & \ast & 0 & 0 \\ & \ast & \ast & \bar{\ast} & 0 & 0 \\ & & \ast & 0 & 0 & 0 \\ & & & \ast & 0 & 0 \\ & & & & \ast & \ast \\ & & & & & \otimes \end{bmatrix}, \quad m=6. \qquad (2.6\text{-}5)$$

(V) **Tetragonal Materials.** Five symmetry planes at $\theta=0$, $\pm\pi/4$, $\pi/2$, and $\psi=\pi/2$.

$$\mathbf{C}=\begin{bmatrix} \ast & \ast & \ast & 0 & 0 & 0 \\ & \ast & \ast & 0 & 0 & 0 \\ & & \ast & 0 & 0 & 0 \\ & & & \ast & 0 & 0 \\ & & & & \ast & 0 \\ & & & & & \ast \end{bmatrix}, \quad m=6. \qquad (2.6\text{-}6)$$

(VI) **Transversely Isotropic (or Hexagonal) Materials.** The symmetry planes are the $x_3=0$ plane and any plane that contains the x_3-axis. The x_3-axis is the axis of symmetry.

$$\mathbf{C}=\begin{bmatrix} \ast & \ast & \ast & 0 & 0 & 0 \\ & \ast & \ast & 0 & 0 & 0 \\ & & \ast & 0 & 0 & 0 \\ & & & \ast & 0 & 0 \\ & & & & \ast & 0 \\ & & & & & \otimes \end{bmatrix}, \quad m=5. \qquad (2.6\text{-}7)$$

(VII) **Cubic Materials.** Nine planes of symmetry whose normals are on the three coordinate axes and on the coordinate planes making an angle $\pi/4$ with the coordinate axes.

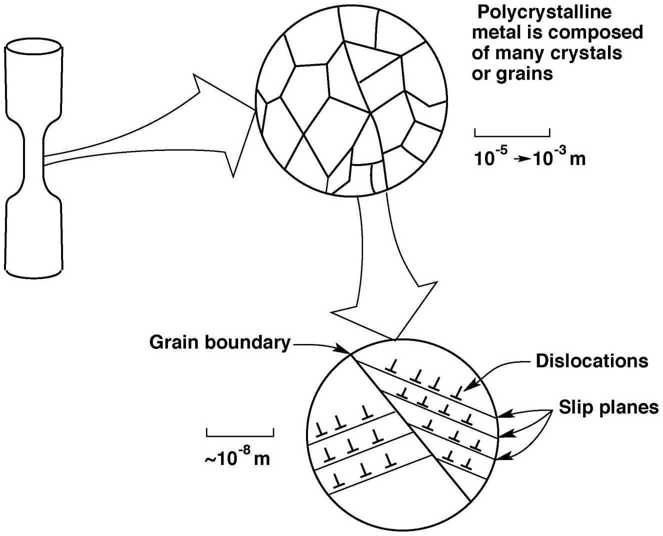
$$\mathbf{C}=\begin{bmatrix} \ast & \ast & \ast & 0 & 0 & 0 \\ & \ast & \ast & 0 & 0 & 0 \\ & & \ast & 0 & 0 & 0 \\ & & & \ast & 0 & 0 \\ & & & & \ast & 0 \\ & & & & & \ast \end{bmatrix}, \quad m=3. \qquad (2.6\text{-}8)$$

(VIII) **Isotropic Materials.** Any plane is a symmetry plane.

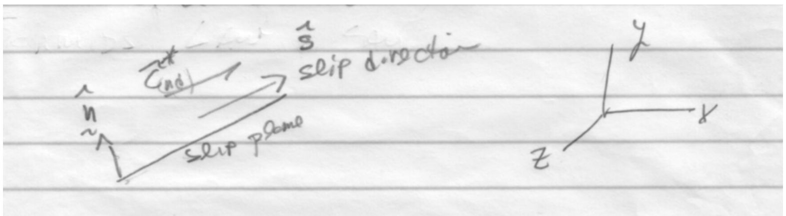
$$\mathbf{C}=\begin{bmatrix} \ast & \ast & \ast & 0 & 0 & 0 \\ & \ast & \ast & 0 & 0 & 0 \\ & & \ast & 0 & 0 & 0 \\ & & & \otimes & 0 & 0 \\ & & & & \otimes & 0 \\ & & & & & \otimes \end{bmatrix}, \quad m=2. \qquad (2.6\text{-}9a)$$

5.9 Crystal Plasticity

- Inelastic deformation on the crystal scale is about the movement of defects through the crystal lattice. The most common defect is the **dislocation** and the most common way for a dislocation to move through the lattice is by glide (slip) on a slip plane in the slip direction. A polycrystalline sample is shown below with the crystals dislocations on the slip systems shown.



- Plasticity happens under the application of an external load (stress). The driving force for dislocation glide is the shear stress that is resolved on the slip plane, $\hat{\mathbf{n}}$, in the slip direction,$\hat{\mathbf{s}}$, as shown below. We'll refer to this shear stress as τ^*_{ns} or just τ^*.



- Just like yielding on the macroscale, when τ^* gets large enough, yielding happens. This is referred to as Schmid's law:

$$\tau^* = \tau_{CRSS} \tag{133}$$

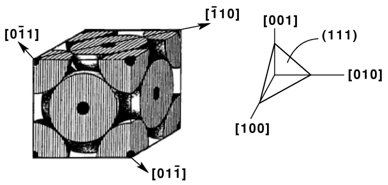
where τ_{CRSS} is the Critically Resolved Shear Stress. So understanding yielding by dislocation glide in a crystal under a general state of stress, σ comes down to determining τ^*, i.e.

$$\tau^* = \hat{\mathbf{s}} \cdot \underline{\boldsymbol{\sigma}} \cdot \hat{\mathbf{n}} = s_i \sigma_{ij} n_j = (\hat{\mathbf{s}} \otimes \hat{\mathbf{n}}) : \underline{\boldsymbol{\sigma}} \tag{134}$$

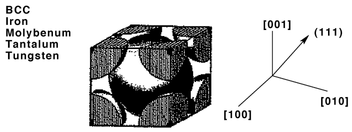
- τ_{CRSS} is a property like macroscopic yield strength.

- The combination of $\hat{\mathbf{n}}$ and $\hat{\mathbf{s}}$ define a "slip system", which are typically known for many classes of crystals. Typically dislocation glide takes place on close packed planes in close packed directions. Slip systems for FCC, BCC and HCP crystal systems are given below
  - The close packed directions in an FCC crystal are the $< 110 >$ family of directions.

Face-centered cubic (FCC) metals



Body-centered cubic (BCC) metals



Close-packed directions: <111> = slip directions

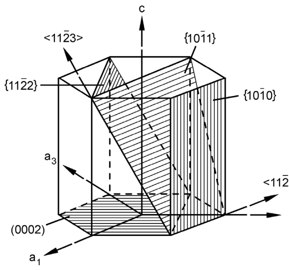


Fig. 2.6. Slip planes and slip directions in the hexagonal α phase

- In the BCC, the $< 111 >$ is the close packed direction but there are no ideally close packed planes. Depending on element, the possible planes are the $\{110\}$, the $\{112\}$ or the $\{123\}$
- Using the four index h,k,i,l Miller Bravais format (h+k+i=0), the potential HCP slip systems are given for titanium in the table below [15]. The basal plane is the ideally close packed plane but to get inelastic extension in the "c" direction, one or more of the other slip systems must activate. These systems typically have a greater τ_{CRSS} values. Twinning (another inelastic deformation mode) is also possible in HCP materials like commercially pure titanium

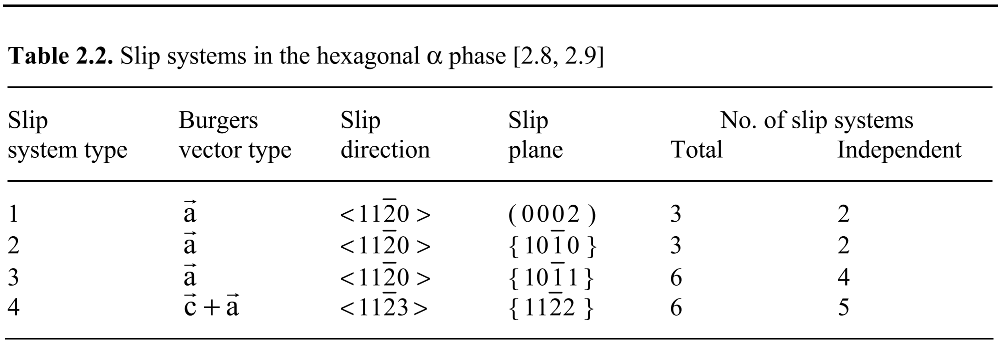


Table 2.2. Slip systems in the hexagonal α phase [2.8, 2.9]

Slip system type	Burgers vector type	Slip direction	Slip plane	No. of slip systems Total	 Independent
1	$\vec{a}$	$<11\bar{2}0>$	(0002)	3	2
2	$\vec{a}$	$<11\bar{2}0>$	$\{10\bar{1}0\}$	3	2
3	$\vec{a}$	$<11\bar{2}0>$	$\{10\bar{1}1\}$	6	4
4	$\vec{c}+\vec{a}$	$<11\bar{2}3>$	$\{11\bar{2}2\}$	6	5

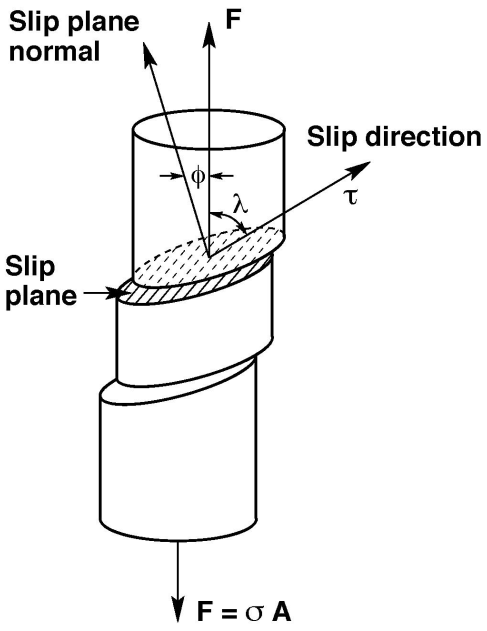
- To determine which slip systems are active, one merely takes the crystal stress (perhaps determined using the elasticity equations in the previous section) and calculates τ^* using Eq. 134.
- If the stress state within the single crystal is uniaxial, a classic derivation for the "Schmid factor" arises. The figure below depicts the single crystal specimen, the slip system and the angles ϕ and λ. Eq. 134 results in

$$\tau^* = \cos\phi\cos\lambda\sigma = m\sigma \tag{135}$$

  where m is defined as the Schmid factor and σ=Load/area is the uniaxial stress in the tension sample.

- The easiest way calculate m is to define a unit vector $\hat{\mathbf{v}}$ in the loading direction, then $\cos\phi = \hat{\mathbf{n}} \cdot \hat{\mathbf{v}}$ and $\cos\lambda = \hat{\mathbf{s}} \cdot \hat{\mathbf{v}}$.
- Considering the slip systems for an FCC crystal:

$$\begin{array}{cccc}
(111) & (\bar{1}11) & (1\bar{1}1) & (11\bar{1}) \\
\hline\hline
[10\bar{1}] & [10\bar{1}] & [10\bar{1}] & [101] \\
[1\bar{1}0] & [0\bar{1}1] & [011] & 011] \\
[1\bar{1}0] & [110] & [110] & [1\bar{1}0]
\end{array} \tag{136}$$



ϕ = angle between the loading axis and the slip plane normal.
λ = angle between the loading axis and the slip direction.
λ and ϕ aren't coplanar.
$\lambda + \phi \neq 90°$

- Let's check a couple Schmid factors
  - For crystal being loading in the [112] direction, calculate m for:
    - the $(111)[10\bar{1}]$ slip system: $\hat{\mathbf{v}} = \frac{1}{\sqrt{6}}[112]$, $\hat{\mathbf{n}} = \frac{1}{\sqrt{3}}[111]$ and $\hat{\mathbf{s}} = \frac{1}{\sqrt{2}}[10\bar{1}]$. so $m = (\hat{\mathbf{s}} \cdot \hat{\mathbf{v}})(\hat{\mathbf{n}} \cdot \hat{\mathbf{v}}) = 0$
    - the $(\bar{1}11)[0\bar{1}1]$ slip system: $\hat{\mathbf{v}} = \frac{1}{\sqrt{6}}[112]$, $\hat{\mathbf{n}} = \frac{1}{\sqrt{3}}[\bar{1}11]$ and $\hat{\mathbf{s}} = \frac{1}{\sqrt{2}}[0\bar{1}1]$. so $m = (\hat{\mathbf{s}} \cdot \hat{\mathbf{v}})(\hat{\mathbf{n}} \cdot \hat{\mathbf{v}}) = \frac{1}{2\sqrt{3}} \cdot \frac{\sqrt{2}}{3} = \frac{\sqrt{6}}{18}$
- Clearly, the slip system with the largest Schmid factor will yield "first".

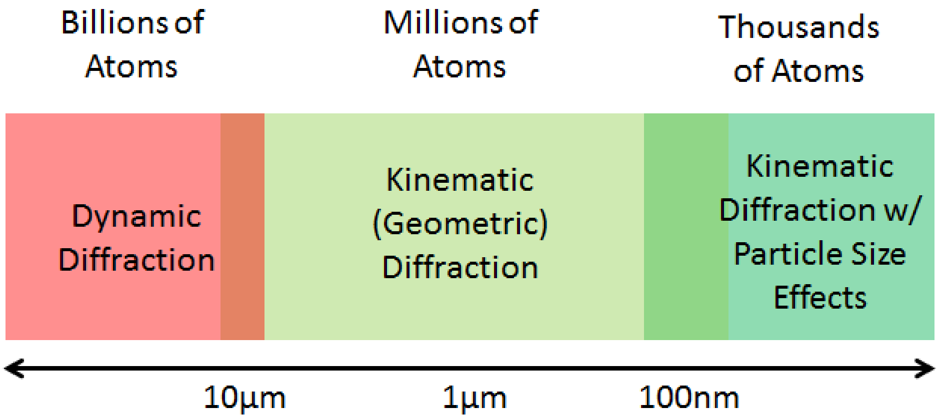
6 Advanced Experiment and Modeling Concepts

We have developed the fundamental relationships for taking diffracted intensity and computing lattice strains and stresses. In this chapter, we present more detailed information on the diffraction model, the x-ray - detector interface and the effects of detector distance and grain size on data. We also present a very continuum mechanically complete analysis that can be used instead of / with the Rosette equations that we developed previously.

6.1 Choice of Diffraction Model

Diffracted intensity shows up as an integer number associated with each pixel on an area detector. A model is required to link the diffraction data to the internal structure of a polycrystal. We have talked about the specifics of kinematic diffraction. In the end, we end up associating a value of diffracted intensity with a particular $\boldsymbol{g}$ vector. In the previous section, we discussed the use of the rosette equations from experimental stress analysis to determine the lattice strain tensor. Here, we present a more complete description that basically blends diffraction with a continuum mechanics description of a polycrystal. We will end up with a relationship that contains both the lattice strain tensor and the grain–averaged lattice reorientation. We also describe the use of data from detectors positioned at various distances from the sample.

- For the next portion of the class, we will be discussing modeling diffracted intensity from deformed crystalline samples
    - Note: Deformed is a relative term, almost all crystalline materials can be treated as deformed when modeling X-ray experiments.
- The first step is to choose our diffraction model.
    - The choice will be dictated by the size of our basic diffracting unit (the size of the unit from which we add the amplitude of the scattered radiation, rather than the intensity)

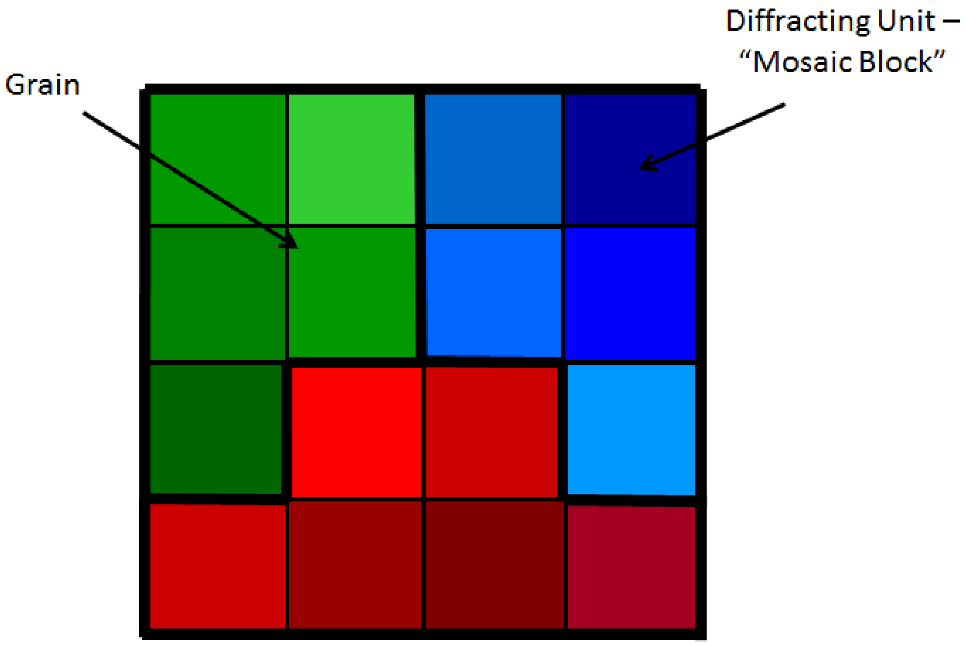


- The two major diffraction models are dynamic and kinematic (geometric) diffraction.
    - Dynamic diffraction models diffraction experiments from crystals that are large enough that the incoming and diffracted X-ray beams interact **strongly** with the electric field inside the crystal ($\boldsymbol{k_i}$ and $\boldsymbol{k_o}$ in the crystal are not equal to $\boldsymbol{k_i}$ and $\boldsymbol{k_o}$ in vacuum)

  - Kinematic diffraction (what we have covered) is a diffraction description in which X-rays interact weakly with the diffracting crystal and the directions of diffracted beams is governed solely by the structure of the crystal and its orientation with respect to the incoming diffracted beam.
  - If the diffracting units are very small ($< 100nm$, nano-grained or heavily cold worked metals), crystallite size effects must be accounted for (see coherent diffraction section)

- The next step is to determine what defines the size of a diffracting units.
  - In our study of kinematic diffraction from a perfect, infinite crystal, we found the diffraction condition to be a δ function. In reality, even perfect crystals have a (very small) finite, angular acceptance (on the order of arc-seconds ($\frac{1}{3600}^{\circ}$)).
  - If neighboring regions of crystal are misoriented more than this **very** small amount, than they can be treated as separate diffracting units.

- So for nearly all materials, even if the grains are very large, we can still think of the crystal being comprised of much smaller diffracting units. These diffracting units are sometimes referred to as *mosaic blocks.*
  - This model is called a 'mosaic block model' and in this model, our material is *ideally imperfect.*



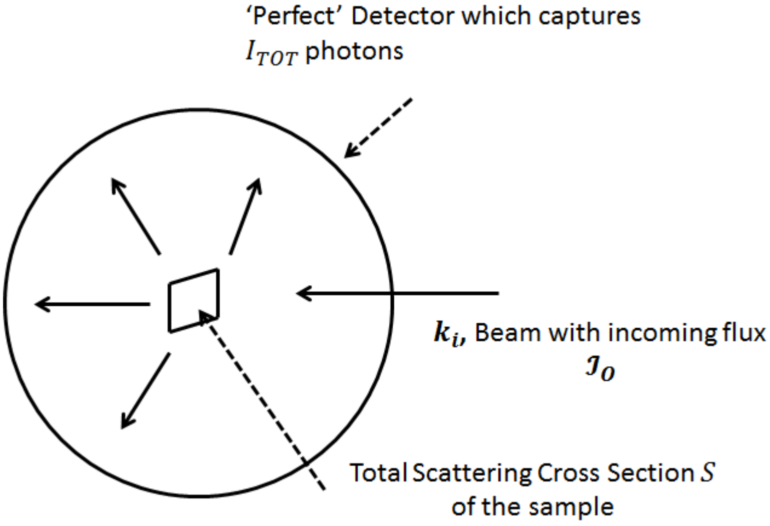
In most crystalline materials, large crystals are comprised of smaller slightly misoriented diffracting units. Different colors represent different orientations.

  - The only times our mosaic block models will not work are for specially grown covalently bonded crystals (think silicon or other semi-conductor materials)

- However, we will find that depending on the *resolution* of our detector, we may able to group our diffracting units together for modeling purposes
  - The resolution of our system is the minimum difference in position or orientation which we can detect.

6.2 The Scattering Cross Section

- We have spent time discussing the conditions in which a sample (crystal) must be oriented for diffracted intensity to be measured.
- We will briefly introduce the formalism used to described scattering from all objects, not just diffracting crystals.
- This is typically done with the introduction of the *differential scattering cross section* of a sample.
  - Portions of the diffraction literature are formulated in terms of the scattering cross section, so we will briefly introduce it.
  - Unfortunately, the standard notation for describing the scattering cross section can be a bit misleading.
- The benefits of describing scattering in terms of a scattering cross section is that the scattering description is independent of detector used and detector distance.
- Lets start by imagining that we have a perfect spherical detector completely surrounding our sample. An X-ray beam of intensity I_0 (units of photons/(area*time))hits our sample and cross our perfect detector we measure scattered photons at a rate of I_{TOT} (units of photons/time).

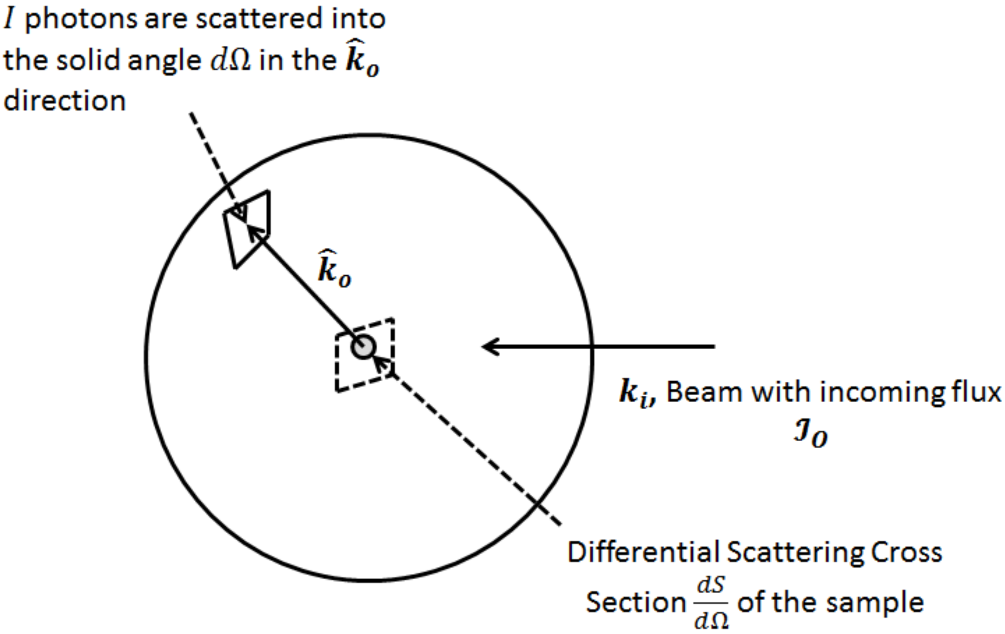


- We will define the ratio of these two quantities as the *total scattering cross section*, S (NOTE: in the literature usually σ is used, we will reserve σ for stress).

$$\frac{I_{TOT}}{I_0} = S(\underline{\boldsymbol{R}}^{L,S}) \tag{137}$$

- It is important to note that the total cross section of the sample changes with sample orientation, which is why we have described S explicitly as a function of the sample orientation.
- The total scattering cross section S has units of area. It can by thought of as hypothetical 'target' size of the sample.

- Next, lets look at the the scattering into the solid angle $d\Omega(\hat{\boldsymbol{k}}_{\boldsymbol{o}})$ of our detector. In the solid angle $d\Omega(\hat{\boldsymbol{k}}_{\boldsymbol{o}})$, I photons/s are measured.



- The differential scattering cross section $(\frac{dS}{d\Omega})$ is then given by:

$$\frac{dS}{d\Omega}(\hat{\boldsymbol{k}}_{\boldsymbol{o}}, \underline{\boldsymbol{R}}^{L,S}) = \frac{I}{I_0} \tag{138}$$

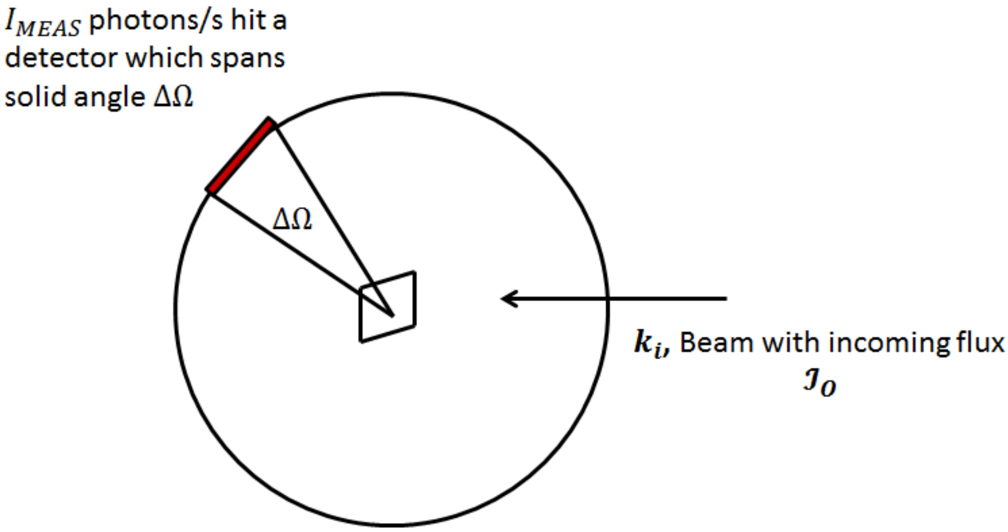
- We can think of the differential scattering cross section, as a portion of our 'target' S which scatters X-rays into the direction $\hat{\boldsymbol{k}}_{\boldsymbol{o}}$.

- By integrating over all of the solid angles of the sphere, we retrieve our total cross section.

$$S(\underline{\boldsymbol{R}}^{L,S}) = \int \frac{dS}{d\Omega}(\hat{\boldsymbol{k}}_{\boldsymbol{o}}, \underline{\boldsymbol{R}}^{L,S}) d\Omega \tag{139}$$

  - NOTE: As mentioned, notation wise $\frac{dS}{d\Omega}$ doesn't make too much sense. Just referring to the differential cross section as dS would probably have been clearer.

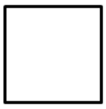
- Lastly, to determine how many photons/second (I_{MEAS}) should scatter into a detector of finite size, all we have to do is integrate over the appropriate solid angle range.



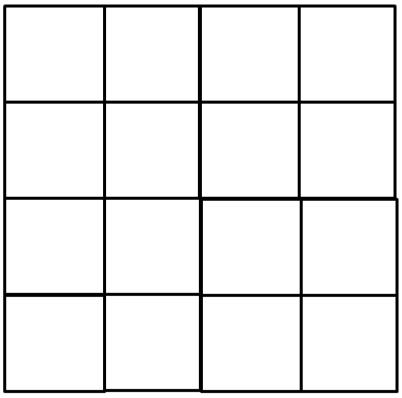
$$I_{MEAS} = \int_{\Delta\Omega} \frac{dS}{d\Omega} d\Omega \tag{140}$$

6.3 X-Ray Detection Geometry

- For our purposes, we will divide detectors into two broad categories, *point detectors* and *area detectors*.
- These terms are colloquial and a bit misleading, all detectors are area detectors.
  - A point detector should be thought of as a small area detector.
  - An area detector should be thought of as a collection of small area detectors.

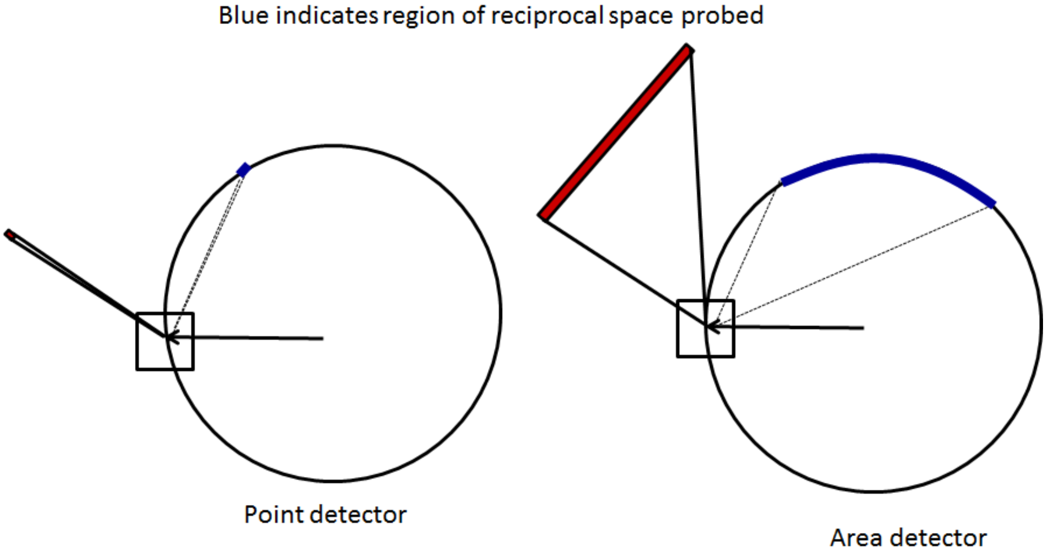


Point detector which spans an area ΔA

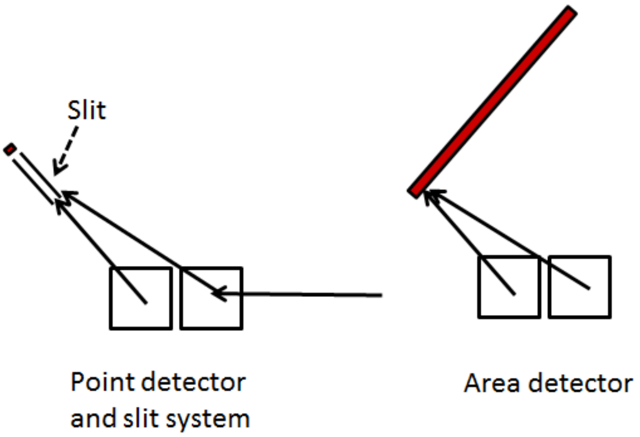


Area detector which spans an area $A = \sum \Delta A$

- Each detection system has its strengths and weaknesses, which we will briefly discuss.
- The primary benefit of an area detector is that a large amount of solid angle is spanned, so large amounts of reciprocal space can be imaged at once.



- While it is fairly straight forward to use slits, to separate scattering from different positions in a sample using a point detector.



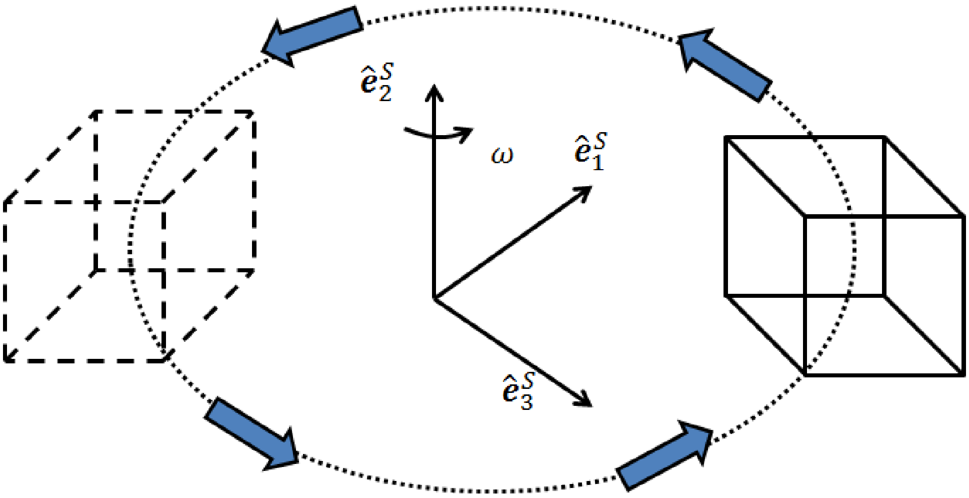
- NOTE: We do not wish to say that the downsides of each detector type can't be overcome (point detectors can moved and slitting systems (conical slits) exist for area detectors). It is just a matter of choice for what is better for the experiment to be conducted.

6.4 Diffracted Intensity from Deformed Crystals

- We will now model the diffracted intensity from a deformed crystal. We have already discussed that we can 'build' a complete crystal from small diffracting units (mosaic block).
- In order to do that, we will first explore how to model a crystal which is precessing about the axis of rotation in a rotating crystal experiment.
- Then we will discuss how to model deformation of the crystal lattice including, stretching of the lattice due to strain and differences of orientation of a diffracting unit with respect to its neighbors.
- Lastly, we will look at how changing the distance from the sample to the detector will change the character of the diffracted intensity that we measure.

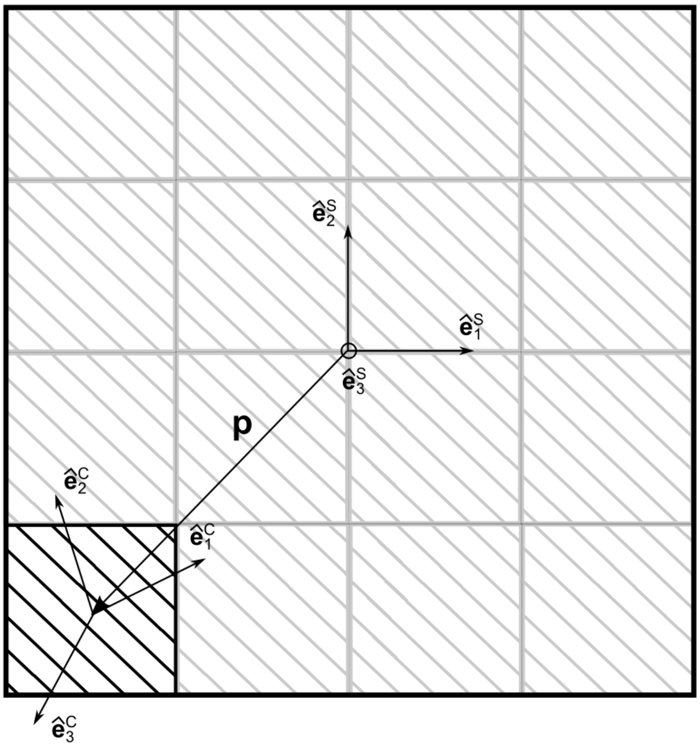
Modeling the position of diffracting units

- Up to this point in the class, we have assumed that our diffracting unit was at the center of the axis of rotation, if this is not true, the crystallite will *precess* about the axis of rotation.

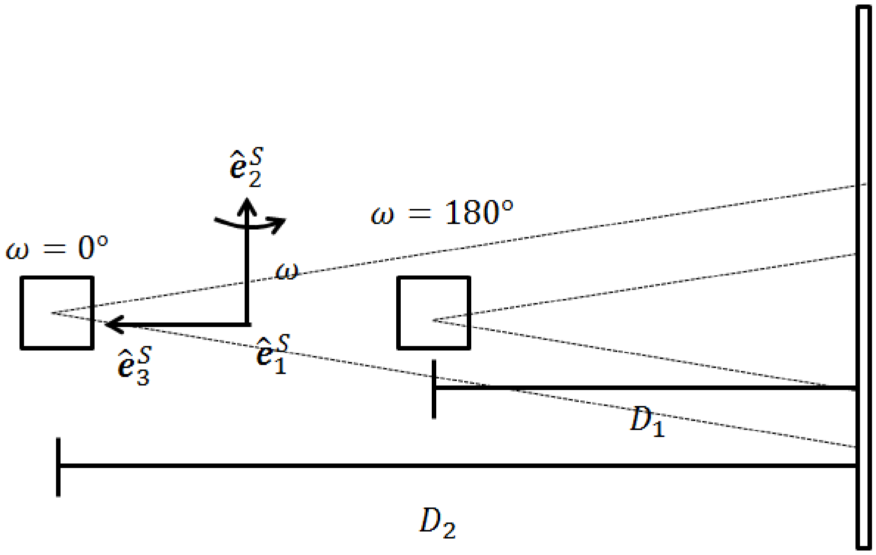


If the center of a diffracting unit is not located on the rotation axis, the crystal will precess as the sample rotates

- If we build a sample from many crystallites, they will not all (all but one won't) be centered at the origin of the sample coordinate system. so when modeling the diffraction from the sample, we must account for the position of all of our crystallites.
- The center of each crystallite will have a position $\boldsymbol{p}$ with respect to origin of the laboratory and sample coordinate systems.

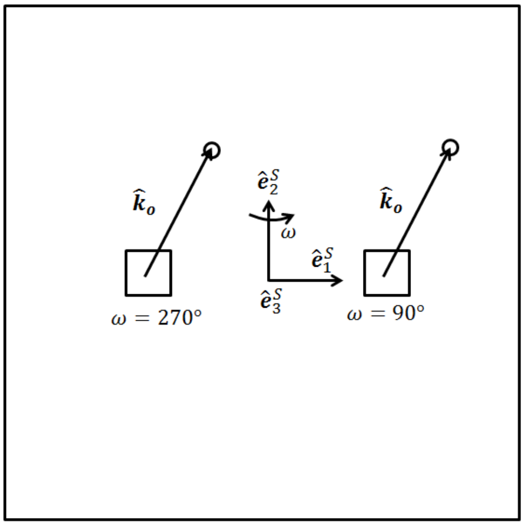


- Precession of the crystallite has two effects:
  - First, the distance from the sample to the detector will change as the sample rotates. This will change the apparent radii upon which diffraction peaks appear on the detector.



As the sample precesses around the rotation axis, diffraction peaks from the same families of lattice planes will appear at different radii on the detector

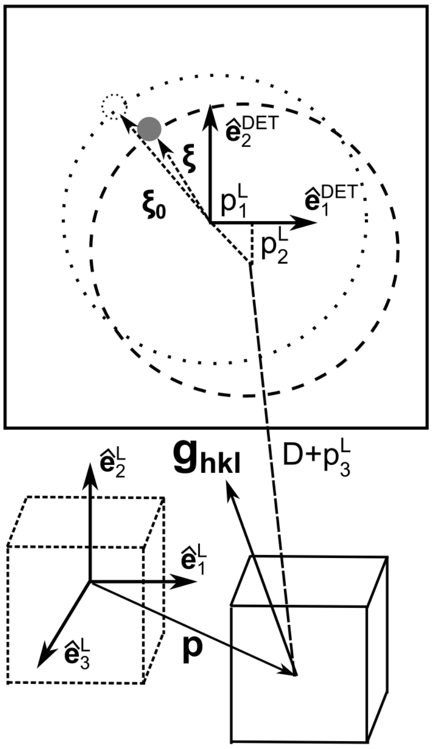
  - Second, as the crystallite precesses, the crystallite translates across the beam shifting diffraction peaks upon the detector.



As the sample precesses around the rotation axis, diffraction peaks will appear to shift on the detector due to translation of the sample

- We will find an expression to account for these effects in a rotating crystal experiment. Our detector will assumed to be a flat plane that is perpendicular to $\hat{e}_3^L$.
  - Note: Equations to account for an arbitrarily tilted detector plane be found in a straight forward manner.

- We will start by finding the intercept ($\boldsymbol{\xi_0}$) of a beam ($\boldsymbol{k_o}$) emitted from the center of the laboratory coordinate system.



- Since we know the beam is traveling along $\boldsymbol{\hat{k}_o}$, intercepts the detector at $\boldsymbol{\xi_0}$, and the detector is a distance D away from the sample. We can solve the set of equations:

$$C\begin{bmatrix}\hat{k}^L_{\boldsymbol{o}1}\\ \hat{k}^L_{\boldsymbol{o}2}\\ \hat{k}^L_{\boldsymbol{o}3}\end{bmatrix}=\begin{bmatrix}\xi_{\mathbf{0}1}\\ \xi_{\mathbf{0}2}\\ -D\end{bmatrix}\tag{141}$$

to find $\boldsymbol{\xi_0}$ where C is a scaling constant.

$$\boldsymbol{\xi}_0=\begin{bmatrix}-(k^L_{o1}/k^L_{o3})D\\ -(k^L_{o2}/k^L_{o3})D\end{bmatrix}\tag{142}$$

- Now we will account for the position $\boldsymbol{p}$ of the crystal. The distance from the sample to detector during the diffraction event is now $D+p^L_3$, and we will translate the the intercept with the detector by the transverse position of the sample p^L_1 and p^L_2.

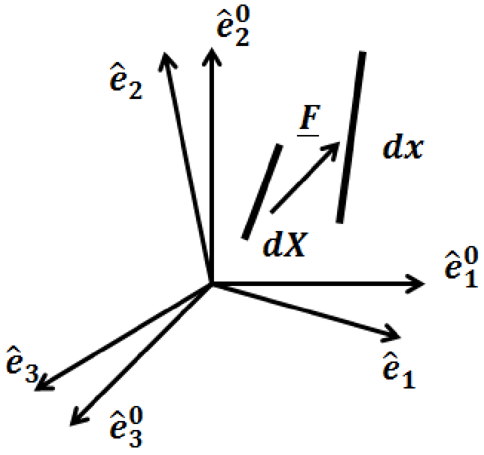
$$\boldsymbol{\xi}=\begin{bmatrix}p^L_1\\ p^L_2\end{bmatrix}+\begin{bmatrix}-(k^L_{o1}/k^L_{o3})(D+p^L_3)\\ -(k^L_{o2}/k^L_{o3})(D+p^L_3)\end{bmatrix}\tag{143}$$

$$\boldsymbol{\xi}=\boldsymbol{\xi}_0+\begin{bmatrix}p^L_1-(k^L_{o1}/k^L_{o3})(p^L_3)\\ p^L_2-(k^L_{o2}/k^L_{o3})(p^L_3)\end{bmatrix}\tag{144}$$

Modeling deformed crystallites

- Before we model a deformed crystallites, we will take a short review of some continuum mechanics kinematics.

- The deformation gradient $\underline{\boldsymbol{F}}$ maps an infinitesimal line segment $\boldsymbol{dX}$ ($dX_A\hat{\boldsymbol{e}}^{\boldsymbol{0}}_A$) from the reference configuration to the current configuration $\boldsymbol{dx}$ ($dx_i\hat{\boldsymbol{e}}_i$) where $\hat{\boldsymbol{e}}^{\boldsymbol{0}}_A$ are the basis vectors of the reference coordinate system and $\hat{\boldsymbol{e}}_i$, the current.



$$\boldsymbol{dx} = \underline{\boldsymbol{F}} \cdot \boldsymbol{dX} = \frac{\boldsymbol{dx}}{\boldsymbol{dX}} \cdot \boldsymbol{dX} \tag{145}$$

  - We note that $\underline{\boldsymbol{F}}$ is a *two point tensor* expressed in two coordinate systems: $\underline{\boldsymbol{F}} = F_{iA}\hat{\boldsymbol{e}}_i\hat{\boldsymbol{e}}^{\boldsymbol{0}}_A$.

- The deformation gradient **rotates** and **stretches** line segments. Using the polar decomposition theorem, we can decompose the deformation gradient into a right stretch tensor $\underline{\boldsymbol{U}}$ ($U_{AB}\hat{\boldsymbol{e}}^{\boldsymbol{0}}_A\hat{\boldsymbol{e}}^{\boldsymbol{0}}_B$) and a rotation **tensor** $\underline{\boldsymbol{R}}$ ($R_{iA}\hat{\boldsymbol{e}}_i\hat{\boldsymbol{e}}^{\boldsymbol{0}}_A$) or a left stretch tensor $\underline{\boldsymbol{V}}$ ($V_{ij}\hat{\boldsymbol{e}}_i\hat{\boldsymbol{e}}_j$) and a rotation **tensor** $\underline{\boldsymbol{R}}$.

$$\underline{\boldsymbol{F}} = \underline{\boldsymbol{R}} \cdot \underline{\boldsymbol{U}} = \underline{\boldsymbol{V}} \cdot \underline{\boldsymbol{R}} \tag{146}$$

  - Note: $\underline{\boldsymbol{V}}$ (V_{ij}) is expressed in terms of the current coordinate system, $\underline{\boldsymbol{U}}$ (U_{AB}) is expressed in terms of the reference coordinate system, and $\underline{\boldsymbol{R}}$ (R_{iA}) is a two point tensor.
  - $\underline{\boldsymbol{R}}$ in this context is not a coordinate transformation!

- With the idea that the deformation gradients maps line segments into a deformed configuration, we will use the deformation gradient to map our initial crystal basis vectors in a crystallite [16].

  - Note: By using a linear mapping, we assume that the deformation is homogeneous in our crystallite. However, the mapping can vary from crystallite to crystallite producing distributions of deformation.

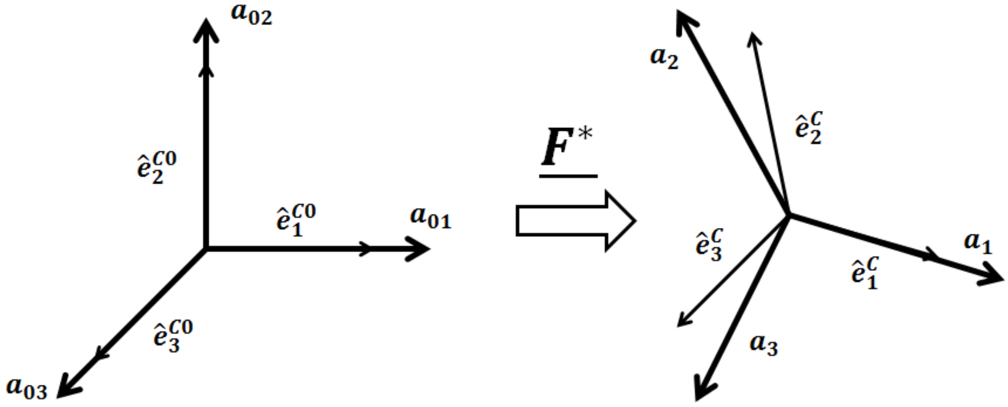
- We will use $\boldsymbol{a_1}$, $\boldsymbol{a_2}$, and $\boldsymbol{a_3}$ to describe the crystal lattice basis vectors in the current configuration (basis: $\hat{\boldsymbol{e}}^{\boldsymbol{C}}_{\boldsymbol{i}}$). The vectors $\boldsymbol{a_{01}}$, $\boldsymbol{a_{02}}$, and $\boldsymbol{a_{03}}$ will described the undeformed crystal lattice vectors in the reference configuration (basis: $\hat{\boldsymbol{e}}^{\boldsymbol{C0}}_{\boldsymbol{A}}$).

- The deformation gradient $\underline{\boldsymbol{F}}^*$ will map the crystal lattice basis vectors from the reference to the current configuration.

$$\boldsymbol{a_1} = \underline{\boldsymbol{F}}^* \cdot \boldsymbol{a_{01}} \tag{147a}$$

$$\boldsymbol{a_2} = \underline{\boldsymbol{F}}^* \cdot \boldsymbol{a_{02}} \tag{147b}$$

$$\boldsymbol{a_3} = \underline{\boldsymbol{F}}^* \cdot \boldsymbol{a_{03}} \tag{147c}$$



- More importantly for modeling a diffraction experiment, we can use the deformation gradient to map the reciprocal lattice basis vectors to the deformed configuration.
- To find out how the reciprocal lattice deforms when the direction lattice is deformed by the deformation gradient $\underline{\boldsymbol{F}}^*$, we will first look at our definition of the reciprocal lattice vector in the current $\boldsymbol{b_1}$ and reference configurations $\boldsymbol{b_{01}}$.

$$\boldsymbol{b_{01}} = \frac{2\pi}{V_0}(\boldsymbol{a_{02}} \times \boldsymbol{a_{03}})$$

$$\boldsymbol{b_1} = \frac{2\pi}{V}(\boldsymbol{a_2} \times \boldsymbol{a_3})$$

$$\boldsymbol{b_1} = \frac{2\pi}{\boldsymbol{a_{01}} \cdot (\boldsymbol{a_{02}} \times \boldsymbol{a_{03}})}(\boldsymbol{a_{02}} \times \boldsymbol{a_{03}})$$

- Using Equation 147

$$\boldsymbol{b_1} = \frac{2\pi}{\underline{\boldsymbol{F}}^* \cdot \boldsymbol{a_{01}} \cdot (\underline{\boldsymbol{F}}^* \cdot \boldsymbol{a_{02}} \times \underline{\boldsymbol{F}}^* \cdot \boldsymbol{a_{03}})}(\underline{\boldsymbol{F}}^* \cdot \boldsymbol{a_{02}} \times \underline{\boldsymbol{F}}^* \cdot \boldsymbol{a_{03}})$$

- We can also recall the identity $\epsilon_{ijk} F^*_{iA} F^*_{jB} F^*_{kC} = J\epsilon_{ABC}$ where $J = Det(\underline{\boldsymbol{F}}^*)$:

$$\boldsymbol{b_1} = \frac{2\pi}{J\boldsymbol{a_{01}} \cdot (\boldsymbol{a_{02}} \times \boldsymbol{a_{03}})}(\underline{\boldsymbol{F}}^* \cdot \boldsymbol{a_{02}} \times \underline{\boldsymbol{F}}^* \cdot \boldsymbol{a_{03}})$$

$$\boldsymbol{b_1} = \frac{2\pi}{JV_0}(\underline{\boldsymbol{F}}^* \cdot \boldsymbol{a_{02}} \times \underline{\boldsymbol{F}}^* \cdot \boldsymbol{a_{03}})$$

- and the identity $\epsilon_{ijk}F^*_{jB}a_{02B}F^*_{kC}a_{03C} = JF^{*(-1)}_{iA}\epsilon_{ABC}a_{02B}a_{03C}$

$$\boldsymbol{b_1} = \frac{2\pi}{JV_0}(J\underline{\boldsymbol{F}}^{*-\boldsymbol{T}} \cdot (\boldsymbol{a_{02}} \times \boldsymbol{a_{03}}))$$

$$\boldsymbol{b_1} = \underline{\boldsymbol{F}}^{*-\boldsymbol{T}} \cdot \frac{2\pi}{V_0}(\boldsymbol{a_{02}} \times \boldsymbol{a_{03}})$$

$$\boldsymbol{b_1} = \underline{\boldsymbol{F}}^{*-\boldsymbol{T}} \cdot \boldsymbol{b_{01}} \tag{148}$$

- Similar relationships hold for $\boldsymbol{b_2}$ ($\boldsymbol{b_2} = \underline{\boldsymbol{F}}^{*-\boldsymbol{T}} \cdot \boldsymbol{b_{02}}$) and $\boldsymbol{b_3}$ ($\boldsymbol{b_3} = \underline{\boldsymbol{F}}^{*-\boldsymbol{T}} \cdot \boldsymbol{b_{03}}$). If the identities used are unfamiliar, review the deformation of area and volume elements in a continuum mechanics reference.

- Now the relationship between a reciprocal lattice vector in the current and reference frame is equal to:

$$\boldsymbol{g} = h\boldsymbol{b_1} + k\boldsymbol{b_2} + l\boldsymbol{b_3}$$

$$\boldsymbol{g} = h\underline{\boldsymbol{F}}^{*-\boldsymbol{T}} \cdot \boldsymbol{b_{01}} + k\underline{\boldsymbol{F}}^{*-\boldsymbol{T}} \cdot \boldsymbol{b_{02}} + l\underline{\boldsymbol{F}}^{*-\boldsymbol{T}} \cdot \boldsymbol{b_{03}}$$

$$\boldsymbol{g} = \underline{\boldsymbol{F}}^{*-\boldsymbol{T}} \cdot \boldsymbol{g_0} \tag{149}$$

  - It is worth reiterating that $\boldsymbol{g}$ is expressed in terms of $\hat{\boldsymbol{e}}_{\boldsymbol{i}}^{\boldsymbol{C}}$ and $\boldsymbol{g_0}$, $\hat{\boldsymbol{e}}_{\boldsymbol{i}}^{\boldsymbol{C0}}$.

- We can examine equation Equation 149 a bit further. Using the left polar decomposition we find that:

$$(\underline{\boldsymbol{F}}^{*-\boldsymbol{1}})^T = (\underline{\boldsymbol{R}}^{*-\boldsymbol{1}} \cdot \underline{\boldsymbol{V}}^{*-\boldsymbol{1}})^T = \underline{\boldsymbol{V}}^{*-\boldsymbol{T}} \cdot (\underline{\boldsymbol{R}}^{*\boldsymbol{T}})^T = \underline{\boldsymbol{V}}^{*-\boldsymbol{1}} \cdot \underline{\boldsymbol{R}}^*$$

therefore

$$\boldsymbol{g} = \underline{\boldsymbol{V}}^{*-\boldsymbol{1}} \cdot \underline{\boldsymbol{R}}^* \cdot \boldsymbol{g_0} \tag{150}$$

- So matching our intuition, the reciprocal lattice rotates in the same manner as the direct lattice, however stretches as the inverse transpose of the direct lattice (this matches what we've seen earlier in the course, if the lattice plane spacing gets bigger, the reciprocal lattice vectors get smaller).

- Lastly, in most crystalline materials during most deformation modes, the stretch of the **lattice** is very small. We can approximate $\underline{\boldsymbol{V}}^*$ as $(\underline{\boldsymbol{I}} + \underline{\boldsymbol{\epsilon}}^*)$ where $\underline{\boldsymbol{\epsilon}}^*$ is the infinitesimal strain tensor expressed in the rotated configuration, so

$$\underline{\boldsymbol{V}}^{*-\boldsymbol{1}} \approx (\underline{\boldsymbol{I}} - \underline{\boldsymbol{\epsilon}}^*) \tag{151}$$

  - This is because $(\underline{\boldsymbol{I}} - \underline{\boldsymbol{\epsilon}}^*) \cdot (\underline{\boldsymbol{I}} + \underline{\boldsymbol{\epsilon}}^*) = \underline{\boldsymbol{I}} - \underline{\boldsymbol{\epsilon}}^{*\boldsymbol{2}} \approx \underline{\boldsymbol{I}} = \underline{\boldsymbol{V}}^{*-\boldsymbol{1}}\underline{\boldsymbol{V}}$, therefore $\underline{\boldsymbol{V}}^{*-\boldsymbol{1}} \approx (\underline{\boldsymbol{I}} - \underline{\boldsymbol{\epsilon}}^*)$.

- Finally,

$$\boldsymbol{g} = (\underline{\boldsymbol{I}} - \underline{\boldsymbol{\epsilon}}^*) \cdot \underline{\boldsymbol{R}}^* \cdot \boldsymbol{g_0} \tag{152}$$

- $\underline{\boldsymbol{\epsilon}}^*$ can be found using the Rosette equations as discussed in the crystal mechanics section (where we project the lattice strain measurements along the current crystal lattice plane normal directions). However, we must take care when interpreting this lattice strain measure when the crystal has significantly rotated. As mentioned, this strain tensor is expressed in the the rotated configuration. We will now look at why we must take care. We will start with the Rosette equations:

$$\epsilon_{nn} = \hat{\boldsymbol{n}} \cdot \underline{\boldsymbol{\epsilon}}^* \cdot \hat{\boldsymbol{n}} \tag{153}$$

- We will now express the lattice plane normal directions in the un-rotated configuration and find that

$$\epsilon_{nn} = \underline{\boldsymbol{R}}^* \cdot \hat{\boldsymbol{n}}_{\boldsymbol{0}} \cdot \underline{\boldsymbol{\epsilon}}^* \cdot \underline{\boldsymbol{R}}^* \cdot \hat{\boldsymbol{n}}_{\boldsymbol{0}}$$

$$\epsilon_{nn} = \hat{\boldsymbol{n}}_{\boldsymbol{0}} \cdot \underline{\boldsymbol{R}}^{*\boldsymbol{T}} \cdot \underline{\boldsymbol{\epsilon}}^* \cdot \underline{\boldsymbol{R}}^* \cdot \hat{\boldsymbol{n}}_{\boldsymbol{0}}$$

- We will define $\underline{\boldsymbol{\epsilon}}_{\boldsymbol{0}}^*$ as the infinitesimal lattice strain in the un-rotated configuration, where

$$\underline{\boldsymbol{\epsilon}}_{\boldsymbol{0}}^* = \underline{\boldsymbol{R}}^{*\boldsymbol{T}} \cdot \underline{\boldsymbol{\epsilon}}^* \cdot \underline{\boldsymbol{R}}^* \tag{154}$$

  and

$$\epsilon_{nn} = \hat{\boldsymbol{n}}_{\boldsymbol{0}} \cdot \underline{\boldsymbol{\epsilon}}_{\boldsymbol{0}}^* \cdot \hat{\boldsymbol{n}}_{\boldsymbol{0}} \tag{155}$$

- What is clear is that

$$\underline{\boldsymbol{\epsilon}}_{\boldsymbol{0}}^* \neq \underline{\boldsymbol{\epsilon}}^* \tag{156}$$

  and we must interpret our lattice strain tensor values accordingly.

- However, we note that if there if there is no reorientation of the lattice ($\underline{\boldsymbol{R}}^* = \underline{\boldsymbol{I}}$) or the reorientation of the lattice is small enough to be neglected (as during most elastic loading):

$$\underline{\boldsymbol{\epsilon}}_{\boldsymbol{0}}^* = \underline{\boldsymbol{\epsilon}}^* = \underline{\boldsymbol{\epsilon}} \tag{157}$$

- In summary, to simulate diffraction from crystallites with deformed lattices, we can simply map the reciprocal lattice vectors into the current configuration and conduct the simulation of the diffraction experiment (as we already have covered previously in the course).

6.5 Diffracted Intensity Distributions on Area Detectors

- We will now bring everything together to look at how diffracted intensity distributions from deformed crystals and polycrystals (they will be treated in a similar manner) will appear on an area detector.

- Returning to equation 143 using which we can calculate the intercept of a diffracted beam with an area detector from a crystallite not at the origin of the sample coordinate system.

$$\boldsymbol{\xi} = \begin{bmatrix} p_1^L \\ p_2^L \end{bmatrix} + \begin{bmatrix} -(k_{o1}^L/k_{o3}^L)(D + p_3^L) \\ -(k_{o2}^L/k_{o3}^L)(D + p_3^L) \end{bmatrix}$$

while remembering that we can model diffraction from a deformed crystallite by deforming the reciprocal lattice:

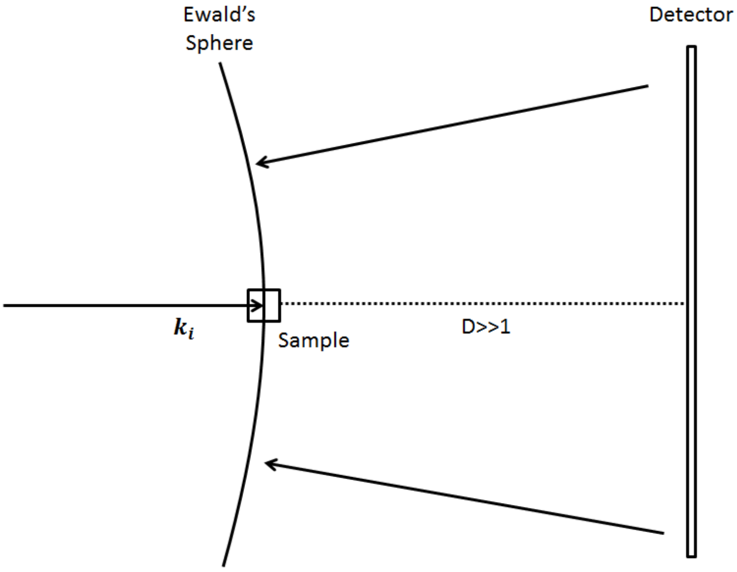
$$\boldsymbol{k_o} = \boldsymbol{k_i} + \boldsymbol{q} = \boldsymbol{k_i} + \boldsymbol{g} = \boldsymbol{k_i} + \underline{\boldsymbol{F}}^{*-\boldsymbol{T}} \cdot \boldsymbol{g_0} \tag{158}$$

- In equation 143, the first term only depends on the position of a crystal during a diffraction event. The second term is dependent on the crystal structure ($\boldsymbol{b_{i0}}$), the orientation of the crystal ($\underline{\boldsymbol{R}}^{S,C}$), and the lattice strain ($\underline{\boldsymbol{\epsilon}}$).
- We can explore the effect of changing the sample to detector distance (D) on where diffraction peaks will hit intercept an area detector with a simple limit analysis.
- As $D \rightarrow \infty$, we see the second term of equation 143 becomes dominant.

$$\boldsymbol{\xi} \approx - \begin{bmatrix} (k^L_{o1}/k^L_{o3})D \\ (k^L_{o2}/k^L_{o3})D \end{bmatrix} \tag{159}$$

$$\boldsymbol{\xi}/D \approx - \begin{bmatrix} (k^L_{o1}/k^L_{o3}) \\ (k^L_{o2}/k^L_{o3}) \end{bmatrix} \tag{160}$$

- In the *far field limit*, there is no influence of the position of a crystallite, and we can interpret the positions of diffraction peaks on the detector being solely due to the crystal lattice.
- We can also interpret our diffracted intensity as a the ‘slice’ of reciprocal space currently in contact with Ewald’s sphere.



In the far field limit, intensity on the detector can be mapped directly to Ewald’s Sphere / reciprocal space

  - NOTE: In most ”far field” experiments, we can still measure average positions of grains in a polycrystal, so the naming of these experiments can be misleading.

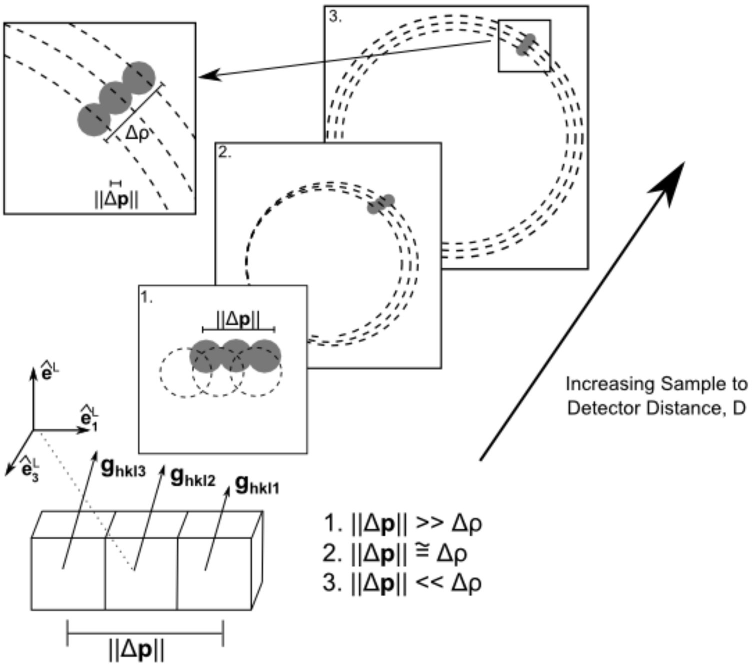
- Now, As $D \rightarrow 0$, we see the first term of equation 143 becomes dominant.

$$\boldsymbol{\xi} \approx \begin{bmatrix} p^L_1 \\ p^L_2 \end{bmatrix} \tag{161}$$

- In the *near field limit*, the intercepts of diffracted intensity with the detector is dominated by the position of the crystallites.
- This enables the use of diffraction to study the shape (topology) of a collection of crystallites.
- Its important to remember that there is no such thing as a perfect near field or far field experiment. The influence of both the crystallite position and the lattice of the crystallite will change where diffracted beams intercept the detector, but it is important to understand which effects are dominant.

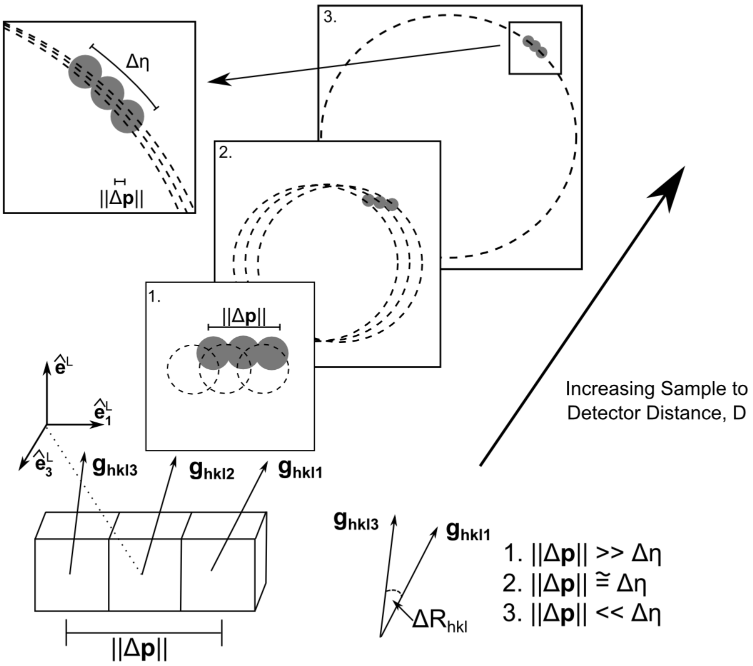
Diffracted intensity from a deformed single crystal

- When measuring the diffracted intensity from an imperfect crystal (in our case modeled as a collection of crystallites), each diffraction peak will have a distribution of diffracted intensity regardless of detector position.
- As discussed, as the detector is moved back, the intercepts of diffracted beams become from crystallites become dominated by the orientation and strain within the lattice (since $\boldsymbol{k_o}$ dominates where a peak will intercept the detector).
- If the collection of crystallites has a distribution of lattice strain, the diffraction peak will spread in the radial direction of the detector in the far field since the variation in lattice plane spacing will cause the crystallites to diffract beams at different 2θ angles.
- The distribution of diffracted intensity from the collection of crystallites therefore transitions from being dominated by the positions of the crystallites in the sample to being dominated by the distribution of strain among the crystallites, which we can see below.



- If the collection of crystallites has a distribution of lattice orientation, the diffraction peak will spread in the azimuthal direction (along Debye rings) of the detector in the far field since the variation in lattice plane orientation will cause reciprocal lattice vectors to intercept Ewald's sphere at different position.

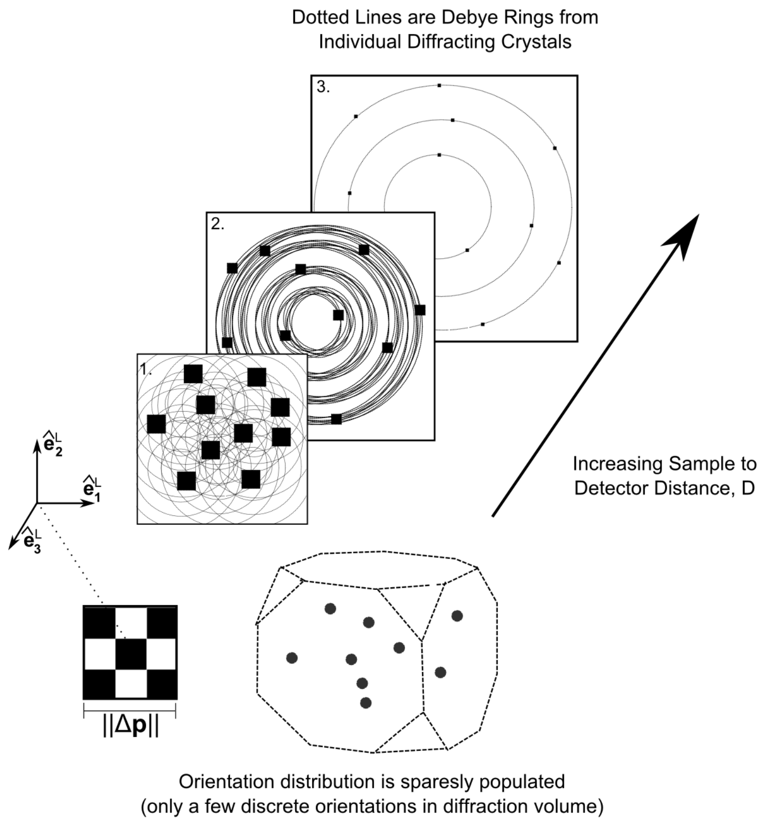
- Again below, we can see the diffracted intensity transitions from being dominated by the positions of the crystallites in the sample to being dominated by the distribution of orientation among the crystallites.



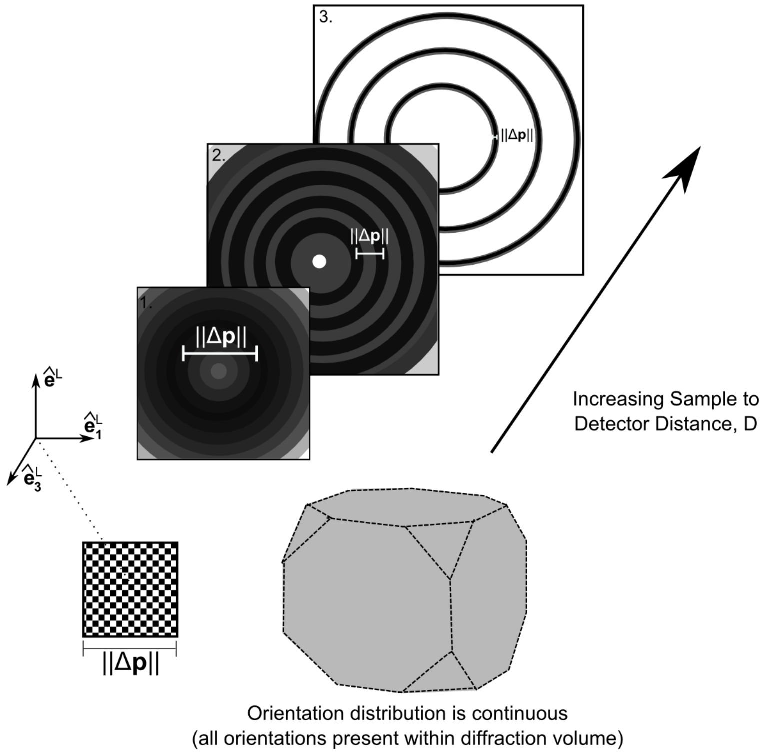
- As crystals become increasingly strained, the size of the distribution of strain and orientation of the crystallites which comprise the crystal become larger, so the peaks tend to grow larger (with a few exceptions).

Diffracted intensity from a polycrystal

- We can also investigate how a polycrystal will diffract using the same model of our sample being composed of diffracting crystallites.
- However, it will be valuable to tie this model to our understanding of orientation space.
- We will start with a crystal with an orientation distribution that has a few regions where crystallites are clustered around an average grain orientation and the rest of the orientation distribution is zero.
- In this case, the diffraction peaks are still easily distinguishable and we can apply the same interpretation of the intensity distributions from each grain in the same manner as the deformed crystal.



- As orientation space becomes more populated (a set of crystallites with all possible orientations is present within the diffraction volume), diffraction peaks begin to overlap.



- In the near field, our diffracted intensity becomes a continuous distribution which decays in the radial direction. It is currently not possibly to extract any quantitative data from diffracted intensity in the near field if distinct peaks can not be discerned.

- In the far field, the diffracted intensity coalesces into distinct filled Debye rings. From this data we can collect *orientation averaged* information about the collection of crystallites that comprise our sample volume.

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