One way to determine crystal structure is to bombard the crystal with X-rays, neutrons or electrons and observe the intensity of the scattered radiation or particles at various angles. One finds that the scattering intensity depends strongly on the wavelength of the incident particle/radiation and the angle at which scattering occurs.

**Bragg Condition**

The early exploration of this scattering behavior regard the crystal lattice as a sequence of parallel planes of lattice sites, each of which reflected the radiation or particles according to standard laws of reflection; For example in a cubic lattice, one possibility would be

\[ n \lambda = 2d \sin \theta \]

where the planes are distance \( d \) apart (this is not necessarily the distance between lattice sites). The outgoing beams will interfere and a peak in intensity will only occur where:

\[ n \lambda = 2d \sin \theta \]

where \( n \) is an integer, and \( \lambda \) the wavelength of the incoming radiation or particle. This is called Bragg's Law and a derivation using simple trigonometry or geometry based on the diagram above is presented in the text in Ch 2.3. The derivation of the Bragg law invokes planes rather than individual atoms and we shall motivate it in terms of scattering from individual atoms within a crystal structure.
Clearly to discuss scattering, we will need to be able to describe planes of lattice sites in crystals.

**Lattice Planes**

Consider a rectangular lattice generated by lattice vectors

\[
\hat{a}_1 = a_1 \hat{x} \\
\hat{a}_2 = a_2 \hat{y} \\
\hat{a}_3 = a_3 \hat{z}
\]

We can illustrate some crystal planes that are parallel to the $z$-axis. All that is required to describe these is a line in the $x$-$y$ plane passing through the origin. This will give a plane passing through the origin others of a similar type can be constructed parallel to this. Thus we can construct:

a) \[\begin{array}{c}
\cdot \\
\cdot \\
\cdot \\
\cdot \\
\cdot \\
\cdot \\
\cdot \\
\cdot \\
\cdot \\
\cdot \\
\end{array}\]

b) \[\begin{array}{c}
\cdot \\
\cdot \\
\cdot \\
\cdot \\
\cdot \\
\cdot \\
\cdot \\
\cdot \\
\cdot \\
\cdot \\
\end{array}\]

c) \[\begin{array}{c}
\cdot \\
\cdot \\
\cdot \\
\cdot \\
\cdot \\
\cdot \\
\cdot \\
\cdot \\
\cdot \\
\cdot \\
\end{array}\]

We will be interested in describing these planes and the distances between parallel planes and we want to do so in terms of the lattice vectors $\hat{a}_1, \hat{a}_2, \hat{a}_3$.

The basic ideas are that

i) any set of parallel planes can be described in terms of a unit vector $\hat{n}$ which is normal to the planes.

ii) we shall construct the normal vectors using $\hat{a}_1, \hat{a}_2, \hat{a}_3$. This involves the realization that any lattice plane is also part of the larger three dimensional lattice.
For example consider a). The plane passing through the origin is:

\[ \hat{n} = \hat{a}_1 \times \hat{a}_3 \]

and a normal to this is \( \hat{n} = \hat{a}_1 \times \hat{a}_3 \). One can see that the plane consists of a two dimensional lattice with lattice vectors \( \hat{a}_1, \hat{a}_3 \).

**Exercise:** Find lattice vectors for the plane of b). Use these to show that a normal is:

\[ \hat{n} = 2 \hat{a}_1 \times \hat{a}_3 + \hat{a}_2 \times \hat{a}_3 \]

In fact, any of the following will also be a normal:

\[ \hat{n} = \lambda \left[ 2 \hat{a}_1 \times \hat{a}_3 + \hat{a}_2 \times \hat{a}_3 \right] \]

**Exercise:** Repeat this for c)

The above illustrate a general fact. A lattice plane in a crystal lattice can be described by the normal:

\[ \hat{n} = \lambda \left[ h \hat{a}_1 \times \hat{a}_3 + k \hat{a}_2 \times \hat{a}_1 + l \hat{a}_3 \times \hat{a}_2 \right] \]

where \( \lambda \) is any real number and \( h, k, l \) are integers which do not all contain the same integer factor. E.g. \( h=4, k=2, l=2 \) is replaced by \( h=2, k=1, l=1 \).

The three numbers \( h, k, l \) are called the **Miller indices** of the plane.
A proof of this fact uses the fact that the plane is a two-dimensional lattice. The lattice vectors which generate the plane \( \vec{u}_1, \vec{u}_2 \) are also position vectors of points in the larger plane. Thus

\[
\vec{u}_1 = n_1 \vec{a}_1 + n_2 \vec{a}_2 + n_3 \vec{a}_3 \\
\vec{u}_2 = m_1 \vec{a}_1 + m_2 \vec{a}_2 + m_3 \vec{a}_3
\]

and the normals to the plane are: 

\[
\lambda (\vec{u}_1 \times \vec{u}_2) = \lambda \left[ \left( n_2 m_3 - n_3 m_2 \right) \vec{a}_1 \times \vec{a}_3 + \left( n_3 m_1 - n_1 m_3 \right) \vec{a}_2 \times \vec{a}_3 \right. \\
\left. + \left( m_1 m_2 - n_2 m_1 \right) \vec{a}_3 \times \vec{a}_2 \right]
\]

which proves the statement.

**Conventional definition of Miller indices**

Ordinarily Miller indices are defined by the intercepts of a lattice plane with the \( x, y, z \) axes. Thus

\[
\vec{r} = x' \hat{x} - y' \hat{y} - z' \hat{z}
\]

Note that the vectors \( \vec{u} = x' \hat{x} - y' \hat{y} \) and \( \vec{v} = x' \hat{x} - z' \hat{z} \) lie in this plane. Thus

\[
\vec{u} \cdot \vec{n} = 0 \Rightarrow \left( \frac{x'}{a_1} \hat{a}_1 - \frac{y'}{a_2} \hat{a}_2 \right) \cdot \vec{n} = 0 \Rightarrow \frac{hx'}{a_1} - \frac{k y'}{a_2} = 0
\]

\[
\vec{v} \cdot \vec{n} = 0 \Rightarrow \left( \frac{x'}{a_1} \hat{a}_1 - \frac{z'}{a_3} \hat{a}_3 \right) \cdot \vec{n} = 0 \Rightarrow \frac{hx'}{a_1} - \frac{l z'}{a_3} = 0
\]

Thus the ratios:

\[
\frac{x'}{a_1} / \frac{y'}{a_2} = \frac{k}{h} \\
\frac{x'}{a_1} / \frac{z'}{a_3} = \frac{l}{h}
\]
Thus we find the threefold ratio:

\[
\left( \frac{x'}{a_1} : \frac{y'}{a_2} : \frac{z'}{a_3} \right) = \left( \frac{1}{h} : \frac{1}{k} : \frac{1}{l} \right)
\]

where \(h, k, l\) are integers.

**Example:** Suppose that \(x' = 3a_1\),

\[
y' = \frac{1}{2}a_2
\]

\[
z' = 5a_3.
\]

Then:

\[
\frac{x'}{a_1} = 3 \quad ; \quad \frac{y'}{a_2} = \frac{1}{2} \quad ; \quad \frac{z'}{a_3} = 5
\]

\[
\Rightarrow \quad \frac{k}{h} = 6 \quad \Rightarrow \quad k = 6h
\]

\[
\Rightarrow \quad \frac{l}{h} = \frac{3}{5} \quad \Rightarrow \quad 5l = 3h
\]

and we choose smallest integers which satisfy this for \(h, k, l\):

- e.g. \(h = 1 \Rightarrow k = 6, l = \frac{3}{5}\) does not work.

- \(h = 5 \Rightarrow k = 30, l = 3\)

\[
\Rightarrow \quad (h, k, l) = (5, 30, 3)
\]

Note that this derivation was only valid for the case where the lattice vectors are rectangular.
Distance between lattice planes

Consider a general lattice. Suppose that the lattice planes are generated by lattice vectors \( \mathbf{u}_1, \mathbf{u}_2 \). Then the density of points in the lattice plane (i.e., the number of points per unit area) in the plane is the inverse of the area of a single primitive cell in the lattice plane. Thus

\[
\text{density of points in lattice plane} = \frac{1}{|\mathbf{u}_1 \times \mathbf{u}_2|}.
\]

On the other hand, the density of points in the 3-dimensional lattice is the inverse of the volume of a primitive cell generated by \( \mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3 \). One can show that this volume is,

\[
|\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)| = |\mathbf{a}_2 \cdot (\mathbf{a}_3 \times \mathbf{a}_1)| = |\mathbf{a}_3 \cdot (\mathbf{a}_1 \times \mathbf{a}_2)|.
\]

Thus,

\[
\text{density of points in 3-d lattice} = \frac{1}{|\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)|}.
\]

If \( d \) is the distance between lattice planes then

\[
\text{density of points in 3-d lattice} = \frac{1}{d} \text{ density of points in lattice plane}
\]

\[d = \frac{|\mathbf{u}_1 \times \mathbf{u}_2|}{|\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)|}
\]

Now we would like to express these in terms of Miller indices. With the vectors \( \mathbf{u}_1, \mathbf{u}_2 \) defined in this way, we note that

\[
\mathbf{u}_1 \times \mathbf{u}_2 = h(\mathbf{a}_2 \times \mathbf{a}_3) + k(\mathbf{a}_3 \times \mathbf{a}_1) + l(\mathbf{a}_1 \times \mathbf{a}_2).
\]

(Also note we can show \( \mathbf{a}_2 \times \mathbf{a}_3, \mathbf{a}_3 \times \mathbf{a}_1, \mathbf{a}_1 \times \mathbf{a}_2 \) are linearly independent, so lowest integers \( h, k, l \) are unique)
Generally it is difficult to compute $|\mathbf{u}_1 \times \mathbf{u}_2|$ unless $\mathbf{\hat{a}}_1, \mathbf{\hat{a}}_2, \mathbf{\hat{a}}_3$ are orthogonal. Thus for a rectangular lattice:

\[
\mathbf{\hat{a}}_1 = a_1 \hat{\mathbf{x}} \\
\mathbf{\hat{a}}_2 = a_2 \hat{\mathbf{y}} \\
\mathbf{\hat{a}}_3 = a_3 \hat{\mathbf{z}}
\]

\[
\Rightarrow \quad \mathbf{\hat{a}}_2 \times \mathbf{\hat{a}}_3 = a_2 a_3 \hat{\mathbf{z}} \\
\mathbf{\hat{a}}_3 \times \mathbf{\hat{a}}_1 = a_3 a_1 \hat{\mathbf{y}} \\
\mathbf{\hat{a}}_1 \times \mathbf{\hat{a}}_2 = a_1 a_2 \hat{\mathbf{x}}
\]

\[
= \quad \mathbf{\hat{u}}_1 \times \mathbf{\hat{u}}_2 = h a_2 a_3 \hat{\mathbf{x}} + k a_3 a_1 \hat{\mathbf{y}} + l a_1 a_2 \hat{\mathbf{z}}
\]

\[
= a_1 a_2 a_3 \left( \frac{h}{a_1} \hat{\mathbf{x}} + \frac{k}{a_2} \hat{\mathbf{y}} + \frac{l}{a_3} \hat{\mathbf{z}} \right). 
\]

But $\mathbf{\hat{a}}_1 \cdot (\mathbf{\hat{a}}_2 \times \mathbf{\hat{a}}_3) = a_1 a_2 a_3$ (Show this!)

and thus:

\[
\frac{1}{d} = \left[ \left( \frac{h}{a_1} \right)^2 + \left( \frac{k}{a_2} \right)^2 + \left( \frac{l}{a_3} \right)^2 \right]^{\frac{1}{2}}.
\]