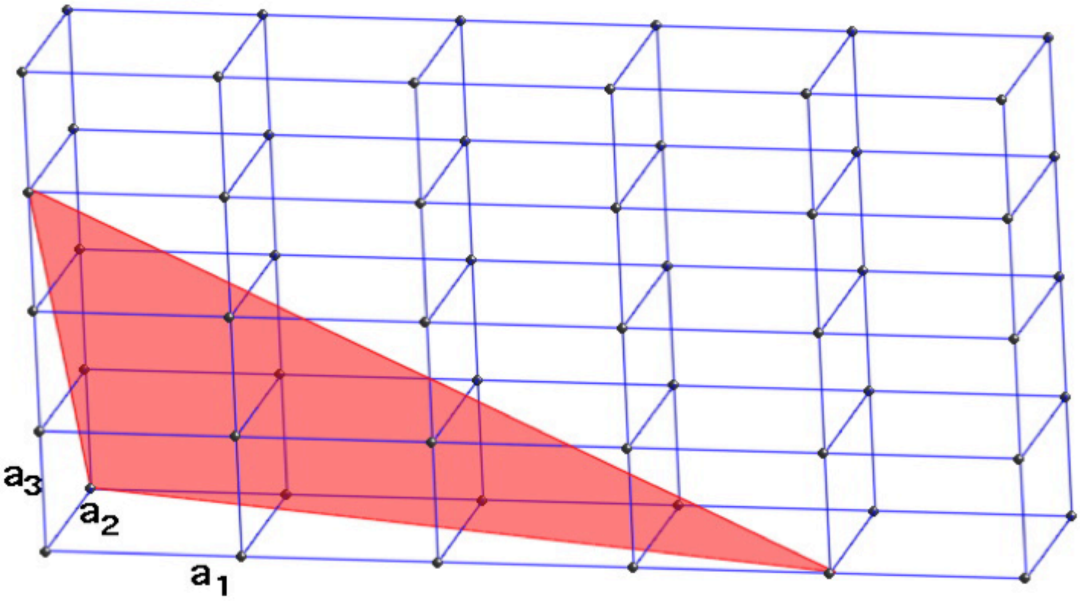
How to characterize crystal faces by reciprocal lattice vectors

The lattice plane, represented below intercepts the three lattice vectors at 4$\mathbf{a}_1$, 1$\mathbf{a}_2$ and 3$\mathbf{a}_3$. In the general case, the integer multiple will be denoted as m_1, m_2 and m_3. Let us suppose also that the normal from the origin to the plane (*i.e.* the distance to the plane) is $\bar{d}$.



To justify the introduction of the reciprocal lattice vectors, we shall show that any normal to any lattice plane is easily expressed in terms of reciprocal lattice vectors. Let us define the normal to the lattice plane by the vector **n** expressed in terms of the reciprocal lattice vectors:

$$\mathbf{n} = n_1\mathbf{a}_1^* + n_2\mathbf{a}_2^* + n_3\mathbf{a}_3^*$$

Our next task is to determine the coefficient n_1, n_2 and n_3 provided the norm of vector **n** is normalized to 1. We can derive the following relations

$$m_1\mathbf{a}_1 \cdot \mathbf{n} = \bar{d} \qquad m_2\mathbf{a}_2 \cdot \mathbf{n} = \bar{d} \qquad m_3\mathbf{a}_3 \cdot \mathbf{n} = \bar{d}$$

If in the first relation we replace vector **n** by its definition, we obtain

$$m_1\mathbf{a}_1 \cdot \mathbf{n} = m_1 n_1 \mathbf{a}_1 \cdot \mathbf{a}_1^* + m_1 n_2 \mathbf{a}_1 \cdot \mathbf{a}_2^* + m_1 n_3 \mathbf{a}_1 \cdot \mathbf{a}_3^* = \bar{d}$$

Among the three scalar products $\mathbf{a}_1 \cdot \mathbf{a}_1^*$, $\mathbf{a}_1 \cdot \mathbf{a}_2^*$, $\mathbf{a}_1 \cdot \mathbf{a}_3^*$ only the first term is equal to 1, the others being zero. We can thus obtain an expression for n_1, which is equal to $\bar{d}/m_1$. We can do the same substitution for n_2 and n_2 and finally we obtain the following expression for the vector **n**

$$\mathbf{n} = \bar{d}\ (\frac{1}{m_1}\mathbf{a}_1^* + \frac{1}{m_2}\mathbf{a}_2^* + \frac{1}{m_3}\mathbf{a}_3^*)$$

To have integer coefficients for the reciprocal vectors, we can modify this equation in the following way. If m is the **smallest common multiple** of m_1, m_2 and m_3, we can modify our equation in the following way

$$\mathbf{n} = \frac{\bar{d}}{m}\ (\frac{m}{m_1}\mathbf{a}^* + \frac{m}{m_2}\mathbf{b}^* + \frac{m}{m_3}\mathbf{c}^*)$$

It turns out that the coefficients m/m_i are all integers, and can thus be replaced by the integers h_i and obtain the following expression for **n:**

$$\mathbf{n} = \frac{\bar{d}}{m}\ (h_1\mathbf{a}_1^* + h_2\mathbf{a}_2^* + h_3\mathbf{a}_3^*) = \frac{\bar{d}}{m}\mathbf{h}$$

The reciprocal vector **h** is thus a sum of integer multiples of the reciprocal unit cell vectors. It is thus a reciprocal lattice vector.

Let us concentrate on the product $\bar{d}/m$. In the figure above illustrating the lattice plane, we can imagine the infinite series of parallel lattice planes, which cover all the lattice nodes. It turns out that the distance between consecutive lattice planes is exactly $\bar{d}/m$. We call this distance d.

The reader can convince himself by drawing a two-dimensional grid with a lattice line intersecting the nodes $3\mathbf{a}_1$ and $4\mathbf{a}_2$. It is easy to see that 12 equidistant parallel lines will appear between that line and the origin after drawing any possible parallel line through each node

We obtain the relation

$$\mathbf{n} = d\mathbf{h}$$

Furthermore, if we take the norms of the vectors, knowing that the norm of vector **n** is equal to 1, we obtain the following relation

$$d_{h_1h_2h_3} = 1/||\mathbf{h}||$$

In other words, any reciprocal lattice vector **h** is normal to a series of parallel lattice planes and the inverse of the norm of the vector gives the distance between the planes. In crystallography, the three indices of the reciprocal vector **h** characterise the normal to the series of planes and are indicated in parenthesis ($h_1h_2h_3$) or more frequently by (*hkl*).

The triplet (*hkl*) is also known as **Miller indices.**

Example

Following our recipe described above, we can now index the face given in the figure above. The m_i is respectively 4,1,3 and the smallest common multiple is 12. The corresponding indices m/m_i in terms of the reciprocal axis are thus (314) which characterise the face.