

Vectors, Matrices and Determinants

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Chapter 2: Tools and tactics for crystals

Here we'll start thinking about using vectors to describe physical structures, especially crystals. To get beyond the basics we'll need two new tools: the scalar triple product, and the reciprocal lattice.

2.1 Planes in orthorhombic crystals

In crystallography, we are often concerned with the vectors that describe the fundamental translational symmetries of the crystal – that is, the directions that we could shift all the atoms in an (infinite, perfect) crystal and just obtain exactly the same structure. Let's first consider just the most basic example: a simple cubic lattice. We will take the lattice constant to be a .

There is a particular kind of notation that it is conventional to use. Three scalars enclosed in square brackets, $[\text{ and }]$, denote a direction. For our simple cubic lattice $[h, k, l]$ means the direction $h\hat{\mathbf{i}} + k\hat{\mathbf{j}} + l\hat{\mathbf{k}}$. However, when we enclose three scalars in regular brackets (and) and omit commas, then we are denoting a plane. By definition $(h \ k \ l)$ is the plane that cuts the three primitive vectors at a/h , a/k and a/l . **Be careful since this is not the usual notation for vectors and planes that we use elsewhere in this course!** The three numbers h , k and l have the name *Miller indices*.

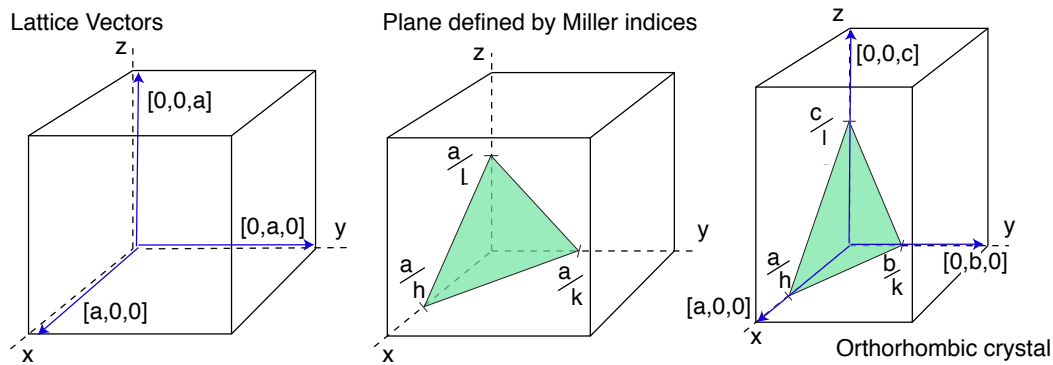


Figure 2.1: Left and middle: vectors and planes in a simple cubic lattice. Right: Orthorhombic crystal.

In addition to a simple cubic lattice, we can immediately use the same ideas to describe a plane in any *orthorhombic* lattice: that is, a generalisation of the cubic case where the atom-to-atom distance can be different in the x , y

and z directions. (To generalise further, to cases where the lattice vectors are not perpendicular to one another, we'll need to use reciprocal lattice vectors – that comes later in these notes!)

Sticking to the cubic case for now, it is straightforward to show that the normal to the plane $(h \ k \ l)$ is in the direction $[h, k, l]$. We simply need to write down two vectors that lie in the plane, and take the cross product.

We know that three particular points in the plane are reached from the origin by the vectors,

$$\mathbf{p}_1 = \frac{a}{h}\hat{\mathbf{i}} \quad \mathbf{p}_2 = \frac{a}{k}\hat{\mathbf{j}} \quad \mathbf{p}_3 = \frac{a}{l}\hat{\mathbf{k}}$$

Warning! notice that there are two quite different “ k ” symbols here. For once, k does not denote the magnitude of $\hat{\mathbf{k}}$ (which is 1 in any case).

A suitable pair of in-plane vectors are, $\mathbf{v}_1 = \mathbf{p}_2 - \mathbf{p}_1$ and $\mathbf{v}_2 = \mathbf{p}_3 - \mathbf{p}_1$. Then

$$\begin{aligned} \mathbf{v}_1 \times \mathbf{v}_2 &= \left(\frac{a}{k}\hat{\mathbf{j}} - \frac{a}{h}\hat{\mathbf{i}} \right) \times \left(\frac{a}{l}\hat{\mathbf{k}} - \frac{a}{h}\hat{\mathbf{i}} \right) \\ &= \frac{a^2}{kl}\hat{\mathbf{j}} \times \hat{\mathbf{k}} - \frac{a^2}{kh}\hat{\mathbf{j}} \times \hat{\mathbf{i}} - \frac{a}{hl}\hat{\mathbf{i}} \times \hat{\mathbf{k}} + \frac{a^2}{h^2}\hat{\mathbf{i}} \times \hat{\mathbf{i}} \\ &= \frac{a^2}{kl}\hat{\mathbf{i}} + \frac{a^2}{kh}\hat{\mathbf{k}} + \frac{a^2}{hl}\hat{\mathbf{j}} + \mathbf{0} \end{aligned}$$

Multiplying through by hkl/a^2 we find

$$\frac{hkl}{a^2}(\mathbf{v}_1 \times \mathbf{v}_2) = h\hat{\mathbf{i}} + k\hat{\mathbf{j}} + l\hat{\mathbf{k}}.$$

Thus the unit normal to the plane, $\hat{\mathbf{n}}$, will be

$$\hat{\mathbf{n}} = \frac{h\hat{\mathbf{i}} + k\hat{\mathbf{j}} + l\hat{\mathbf{k}}}{\sqrt{h^2 + k^2 + l^2}}.$$

Finally we note that another convention in the crystallography field is to put a bar above a number, or symbol, in order to denote a minus sign. So, the plane $(a \ -b \ c)$ is more properly written $(a \ \bar{b} \ c)$.

Examples of Miller indices:

Sketch some examples here. A great free resource is the page at wikipedia, https://en.wikipedia.org/wiki/Miller_index#/media/File:Miller_Indices_Felix_Kling.svg

2.2 Scalar triple product

The scalar triple product is a way to obtain a single scalar number from three vectors. It is simply a combination of the dot product and the cross product concepts that we have met already. We write the scalar triple product as

$$\mathbf{a} \cdot (\mathbf{b} \times \mathbf{c})$$

where the brackets are to stress that we must first take the cross product (but of course this is obvious, since if we began by taking the dot product $\mathbf{a} \cdot \mathbf{b}$, we would then have to take the cross product of a scalar with a vector: impossible!).

Swapping the order of the dot product will make no difference. However, we know that changing the order of a cross product will give an overall minus sign. So:

$$\mathbf{a} \cdot (\mathbf{b} \times \mathbf{c}) = (\mathbf{b} \times \mathbf{c}) \cdot \mathbf{a} \quad \mathbf{a} \cdot (\mathbf{b} \times \mathbf{c}) = -\mathbf{a} \cdot (\mathbf{c} \times \mathbf{b})$$

However, an important property of the scalar triple product is that we can reorder the vectors in a cyclic way. So,

$$\mathbf{a} \cdot (\mathbf{b} \times \mathbf{c}) = \mathbf{b} \cdot (\mathbf{c} \times \mathbf{a}) = \mathbf{c} \cdot (\mathbf{a} \times \mathbf{b})$$

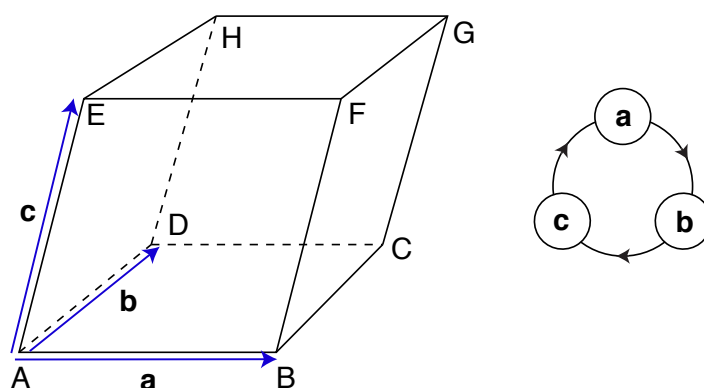


Figure 2.2: Left: A parallelepiped. Right: cyclic rule.

remembering the cyclic construction. The way to prove this is to notice that the scalar triple product is really just the volume of a certain solid: the parallelepiped with edges parallel to $\mathbf{a}$, $\mathbf{b}$ and $\mathbf{c}$.

Consider the Figure (2.2). Note that the sides are just parallelograms, and as we noted earlier the area is therefore given by the magnitude of the cross product between the edge vectors. So, in particular

$$\text{area of side } ABCD = |\mathbf{a} \times \mathbf{b}|$$

Then the volume of the parallelepiped must be, the area of the side multiplied by the perpendicular height (can you convince yourself why this is?). But

$$\text{perpendicular height} = |\mathbf{c}| \cos(\theta)$$

where θ is the angle between $\mathbf{c}$ and the normal to base $ABCD$. But then since $\mathbf{a} \times \mathbf{b} = |\mathbf{a} \times \mathbf{b}| \hat{\mathbf{n}}$, we can simply write

$$\text{volume of parallelepiped } ABCD = |\mathbf{a} \times \mathbf{b}| |\mathbf{c}| \cos(\theta) = \mathbf{c} \cdot (\mathbf{a} \times \mathbf{b})$$

Something to check here: as we have set up our vectors $\mathbf{a}$, $\mathbf{b}$ and $\mathbf{c}$, does the normal point into the volume (so that the final dot product will give us something positive)? Using the right hand rule, we see that it does.

Now the important point is that we can repeat the argument above by finding the area of another side of the parallelepiped, and getting the perpendicular width/depth from that side. Thus, it must follow that

$$\mathbf{a} \cdot (\mathbf{b} \times \mathbf{c}) = \mathbf{b} \cdot (\mathbf{c} \times \mathbf{a}) = \mathbf{c} \cdot (\mathbf{a} \times \mathbf{b}).$$

The restriction to this cyclic ordering comes from the need to make sure the cross product vector is pointing into the volume, according to the right hand rule, in each case.

Finally, let's notice that if we take the triple product of $\mathbf{a}$, $\mathbf{b}$ and $\mathbf{b}$ (that is, $\mathbf{b}$ appearing twice), then the result must be zero.

$$\mathbf{a} \cdot (\mathbf{b} \times \mathbf{b}) = \mathbf{b} \cdot (\mathbf{a} \times \mathbf{b}) = 0.$$

Why?

2.2.1 Finding the triple product via determinant method

We saw before that a helpful method for finding the cross product is to write it as a 'determinant':

$$\begin{aligned} \mathbf{b} \times \mathbf{c} &= \begin{vmatrix} \hat{\mathbf{i}} & \hat{\mathbf{j}} & \hat{\mathbf{k}} \\ b_x & b_y & b_z \\ c_x & c_y & c_z \end{vmatrix} \\ &= \begin{vmatrix} b_y & b_z \\ c_y & c_z \end{vmatrix} \hat{\mathbf{i}} - \begin{vmatrix} b_x & b_z \\ c_x & c_z \end{vmatrix} \hat{\mathbf{j}} + \begin{vmatrix} b_x & b_y \\ c_x & c_y \end{vmatrix} \hat{\mathbf{k}} \\ &= (b_y c_z - b_z c_y) \hat{\mathbf{i}} - (b_x c_z - b_z c_x) \hat{\mathbf{j}} + (b_x c_y - b_y c_x) \hat{\mathbf{k}} \end{aligned}$$

Now we can take the dot product with a third vector $\mathbf{a} = a_x \hat{\mathbf{i}} + a_y \hat{\mathbf{j}} + a_z \hat{\mathbf{k}}$ to obtain,

$$(\mathbf{b} \times \mathbf{c}) \cdot \mathbf{a} = (b_y c_z - b_z c_y) a_x - (b_x c_z - b_z c_x) a_y + (b_x c_y - b_y c_x) a_z.$$

But this means that we can just write the scalar triple product as

$$(\mathbf{b} \times \mathbf{c}) \cdot \mathbf{a} = \mathbf{a} \cdot (\mathbf{b} \times \mathbf{c}) = \begin{vmatrix} a_x & a_y & a_z \\ b_x & b_y & b_z \\ c_x & c_y & c_z \end{vmatrix}$$

...which is a nice compact way to remember it.

Example

2.2.2 Equation of a plane, given two lines and a point

Suppose that we are told that a vector, $\mathbf{a}$, is the position vector of some point in a plane, and that vectors $\mathbf{b}$ and $\mathbf{c}$ are displacements lying within the plane. How can we obtain the equation for that plane?

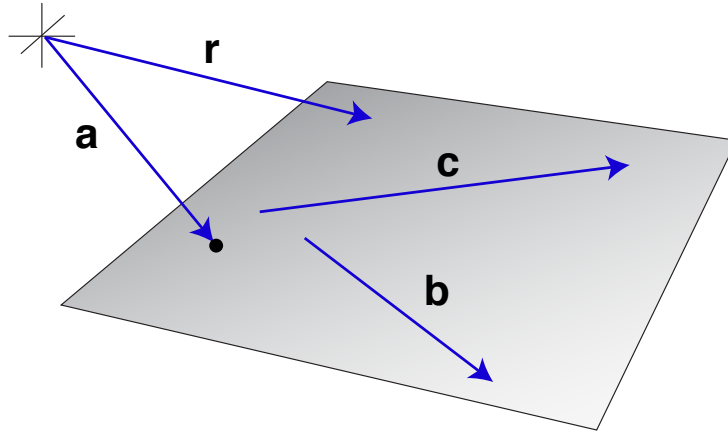


Figure 2.3: A plane defined by $\mathbf{a}$, $\mathbf{b}$ and $\mathbf{c}$.

Well the two vectors in the plane allow us to get the normal vector:

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

and we remember that one kind of equation for a plane is

$$\mathbf{r} \cdot \hat{\mathbf{n}} = c.$$

To find c we can just feed in $\mathbf{r} = \mathbf{a}$, so $\mathbf{r} \cdot \hat{\mathbf{n}} = \mathbf{a} \cdot \hat{\mathbf{n}}$, or more explicitly,

$$\mathbf{r} \cdot \frac{\mathbf{b} \times \mathbf{c}}{|\mathbf{b} \times \mathbf{c}|} = \mathbf{a} \cdot \frac{\mathbf{b} \times \mathbf{c}}{|\mathbf{b} \times \mathbf{c}|}.$$

Note that the right hand side of the expression above is just the distance from the origin. We can tidy up our equation for the plane by writing

$$\mathbf{r} \cdot (\mathbf{b} \times \mathbf{c}) = \mathbf{a} \cdot (\mathbf{b} \times \mathbf{c}),$$

although of course now the RHS is not the distance-to-origin anymore.

2.2.3 Linear independence

Consider two non-parallel vectors $\mathbf{a}$ and $\mathbf{b}$. We know that if we create a new vector $\mathbf{c}$ by some combination of the original two, i.e. $\mathbf{c} = \alpha\mathbf{a} + \beta\mathbf{b}$, then $\mathbf{c}$ must lie in a certain plane: the plane containing the origin and in which $\mathbf{a}$ and $\mathbf{b}$ lie.

Because of this constraint, we say that $\mathbf{c}$ is dependent on (or, “not independent of”) the vectors $\mathbf{a}$ and $\mathbf{b}$. Clearly, we could swap to thinking of $\mathbf{a}$ and $\mathbf{c}$ as our fundamental vectors, and then regard $\mathbf{b}$ as depending on these two. So the key point is that $\mathbf{a}$, $\mathbf{b}$ and $\mathbf{c}$, as a group, are not independent of each other. You could form any one of them by combinations of the other two.

In order for a vector $\mathbf{c}$ to be independent of $\mathbf{a}$ and $\mathbf{b}$, it must not lie in their plane: that is, it must have some component pointing out of the plane containing $\mathbf{a}$ and $\mathbf{b}$. But, this is just the same as saying that the volume of the parallelepiped with edges $\mathbf{a}$, $\mathbf{b}$ and $\mathbf{c}$ must not be zero, or

$$\mathbf{a} \cdot (\mathbf{b} \times \mathbf{c}) \neq 0 \quad \text{for independent } \mathbf{a}, \mathbf{b}, \mathbf{c}.$$

2.2.4 Distance between two lines

This is a calculation that is very complex without the use of vectors! But by using vectors it becomes beautifully simple. Consider two lines, call them $\mathbf{r}_1 = \mathbf{p}_1 + \lambda_1\mathbf{v}_1$ and $\mathbf{r}_2 = \mathbf{p}_2 + \lambda_2\mathbf{v}_2$. We want to know the shortest distance between them.

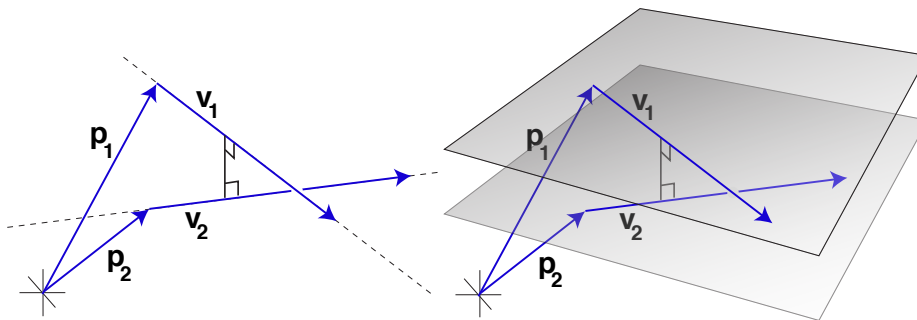


Figure 2.4: The distance between two lines.

First, consider the line connecting the nearest two points. This line is perpendicular to both lines (can you see that?). Now imagine a couple of parallel planes, one containing the first line, and one containing the other. Although there are an infinity of planes that contain a given line, by requiring

that these two planes are parallel we are making them unique. The vector that is normal to the planes (to both of them since they are parallel) is just

$$\hat{\mathbf{n}} = \frac{1}{|\mathbf{v}_1 \times \mathbf{v}_2|} \mathbf{v}_1 \times \mathbf{v}_2$$

Now we can see that all we need to do, is to write down **any** vector going from some point in line 1 to some point in line 2, and then find the component of this vector that is perpendicular to the planes. Of course we will choose the vector $\mathbf{p}_1 - \mathbf{p}_2$, and then

$$\text{distance} = |\hat{\mathbf{n}} \cdot (\mathbf{p}_1 - \mathbf{p}_2)|$$

where we've taken the absolute value since the component might be negative.

Example

2.3 Reciprocal lattice

Earlier we considered the basis vectors of a cubic lattice. Now we will drop the assumption that it is cubic, and consider a general lattice. Suppose that $\mathbf{a}$, $\mathbf{b}$ and $\mathbf{c}$ are the basis vectors of this lattice. Then we write the reciprocal lattice vectors as $\mathbf{a}^*$, $\mathbf{b}^*$ and $\mathbf{c}^*$ and define them by

$$\mathbf{a}^* = \frac{\mathbf{b} \times \mathbf{c}}{\mathbf{a} \cdot (\mathbf{b} \times \mathbf{c})} \quad \mathbf{b}^* = \frac{\mathbf{c} \times \mathbf{a}}{\mathbf{a} \cdot (\mathbf{b} \times \mathbf{c})} \quad \mathbf{c}^* = \frac{\mathbf{a} \times \mathbf{b}}{\mathbf{a} \cdot (\mathbf{b} \times \mathbf{c})}.$$

Notice the cyclic pattern here: we see sequences like $a = bc$, $b = ca$, $c = ab$. Also note that we could reorder the denominators so that they reflect the

cross product above, so e.g. we might write the denominator of $\mathbf{b}^*$ as $\mathbf{b} \cdot (\mathbf{c} \times \mathbf{a})$ if we want.

The reciprocal lattice vectors have several powerful uses. First let's confirm two basic properties:

$$\mathbf{a} \cdot \mathbf{a}^* = 1 \quad \mathbf{b} \cdot \mathbf{b}^* = 1 \quad \mathbf{c} \cdot \mathbf{c}^* = 1$$

but

$$\mathbf{a} \cdot \mathbf{b}^* = 0 \quad \text{and so with all other combos.}$$

Check that this is true. Is it always possible to find these vectors? Well it will be provided that the original vectors are non-coplanar, i.e. provided $\mathbf{a} \cdot (\mathbf{b} \times \mathbf{c}) \neq 0$. Otherwise, our expressions correspond to infinities.

Example

2.3.1 Resolving a vector into three parts

Suppose that we have some vector $\mathbf{v}$ and we want to resolve it into three parts, parallel to three particular vectors $\mathbf{a}$, $\mathbf{b}$ and $\mathbf{c}$. Given that these vectors are not coplanar, this will be possible – but how to do it?

$$\mathbf{v} = v_a \mathbf{a} + v_b \mathbf{b} + v_c \mathbf{c}$$

Remember that if we were asking for the usual Cartesian decomposition, i.e. $\mathbf{v} = v_x \hat{\mathbf{i}} + v_y \hat{\mathbf{j}} + v_z \hat{\mathbf{k}}$, then we could get at any of those coefficients just by doing the dot product with the appropriate unit vector, e.g. $\mathbf{v} \cdot \hat{\mathbf{i}} = v_x$. The property that allows us to do this, is that $\hat{\mathbf{i}}$ is orthogonal to the other two components: $\hat{\mathbf{i}} \cdot \hat{\mathbf{j}} = \hat{\mathbf{i}} \cdot \hat{\mathbf{k}} = 0$.

But we've just seen that the reciprocal lattice vectors $\mathbf{a}^*$, $\mathbf{b}^*$, $\mathbf{c}^*$ have exactly this property with respect to the general vectors $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$! Thus for example,

$$\mathbf{v} \cdot \mathbf{a}^* = (v_a \mathbf{a} + v_b \mathbf{b} + v_c \mathbf{c}) \cdot \mathbf{a}^* = v_a$$

So summarising,

$$v_a = \frac{\mathbf{v} \cdot (\mathbf{b} \times \mathbf{c})}{\mathbf{a} \cdot (\mathbf{b} \times \mathbf{c})} \quad v_b = \frac{\mathbf{v} \cdot (\mathbf{c} \times \mathbf{a})}{\mathbf{a} \cdot (\mathbf{b} \times \mathbf{c})} \quad v_c = \frac{\mathbf{v} \cdot (\mathbf{a} \times \mathbf{b})}{\mathbf{a} \cdot (\mathbf{b} \times \mathbf{c})}.$$

Examples

2.3.2 Solving simultaneous equations

Let's think about the problem of solving for three variables, x , y and z , given three linear equations. One way to write the equations would be,

$$\mathbf{r} \cdot \mathbf{a} = A \quad \mathbf{r} \cdot \mathbf{b} = B \quad \mathbf{r} \cdot \mathbf{c} = C$$

where we'll use $\mathbf{r} = x\hat{\mathbf{i}} + y\hat{\mathbf{j}} + z\hat{\mathbf{k}}$ and we'll select the vectors and constants appropriately. So for example, if the first equation we are given is $4x - 3y + 6z = \frac{2}{3}$ then we will write $\mathbf{a} = 4\hat{\mathbf{i}} - 3\hat{\mathbf{j}} + 6\hat{\mathbf{k}}$ and $A = \frac{2}{3}$.

Thus we can write the equations in vector form. What kind of equations are these, in geometrical terms? They are the equations for three planes (though, be careful because the normals $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$ are not unit vectors, i.e. their magnitude has not been fixed to 1). So, solving them is the same as **finding the intersection of 3 planes**. But how to do it?

We need only notice that, if $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$ are non-coplanar (which they must be or else we would not have three independent equations), then the three reciprocal lattice vectors $\mathbf{a}^*$, $\mathbf{b}^*$, $\mathbf{c}^*$ exist and are non-coplanar. Then, they are also perfectly suitable for expressing $\mathbf{r}$. So we can choose to write

$$\mathbf{r} = \alpha\mathbf{a}^* + \beta\mathbf{b}^* + \gamma\mathbf{c}^*$$

Does that help? It does, as soon as we think about $\mathbf{r} \cdot \mathbf{a}$ in this new decomposition. Because

$$\mathbf{r} \cdot \mathbf{a} = \alpha \quad \text{but from above} \quad \mathbf{r} \cdot \mathbf{a} = A$$

So we conclude that $\alpha = A$ and similarly $\beta = B$, $\gamma = C$. Therefore, as soon as we have found the reciprocal lattice vectors, we can immediately write down the complete solution:

$$\mathbf{r} = A\mathbf{a}^* + B\mathbf{b}^* + C\mathbf{c}^*$$

All we need is for those reciprocal lattice vectors to exist, which we know means that $\mathbf{a} \cdot (\mathbf{b} \times \mathbf{c}) \neq 0$.

2.3.3 The normal to plane ($h \ k \ l$)

As we noted earlier, in crystallography we often deal with lattice vectors: these are the displacements which would shift the entire 3D lattice such that it ends up 'on top' of itself again.

Remember that in crystallographic notation, a plane is denoted by three integers in regular brackets, like ($h \ k \ l$). Normally there are no commas used,

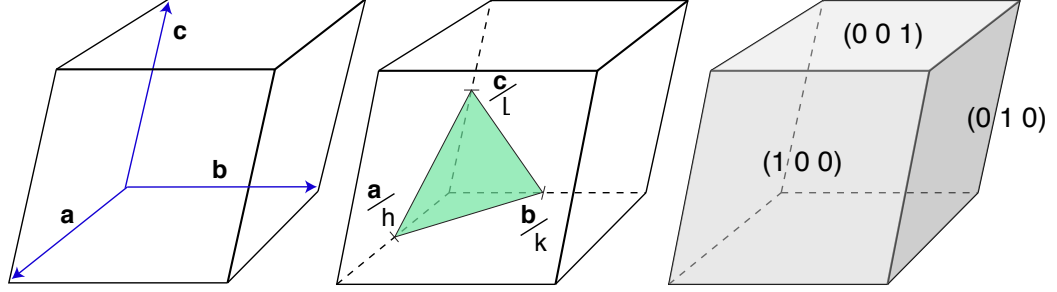


Figure 2.5: Left: A general unit cell with lattice vectors $\mathbf{a}$, $\mathbf{b}$ and $\mathbf{c}$. Middle: A plane with Miller indices (hkl) . Right: The planes (100) , (010) and (001) .

and a bar above a number indicates a negative, i.e. $-2 = \bar{2}$. These three numbers, called the Miller indices, correspond to where the plane cuts the basis vectors $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$.

Meanwhile, if we see three numbers in square brackets, like $[h \ k \ l]$, then this denotes a direction; specifically, the direction of the vector $h\mathbf{a} + k\mathbf{b} + l\mathbf{c}$. Remember that this k is just some variable, not related to $\hat{\mathbf{k}}$. It's a potentially confusing double use of the symbol!

Now that we have introduced the scalar triple product, from Figure 2.5 we can also notice that:

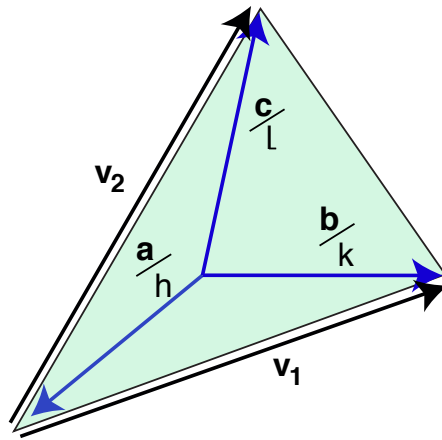
Volume of unit cell formed by $\mathbf{a}$, $\mathbf{b}$ and $\mathbf{c}$ is simply $\mathbf{a} \cdot (\mathbf{b} \times \mathbf{c})$.

(Since this is precisely the volume of such a parallelepiped; see Fig. 2.2).

Previously, we considered the simple cubic lattice, where the basis vectors are $a\hat{\mathbf{i}}$, $a\hat{\mathbf{j}}$, $a\hat{\mathbf{k}}$. We showed that in this case the normal to the plane (hkl) is in the direction of the vector $h\hat{\mathbf{i}} + k\hat{\mathbf{j}} + l\hat{\mathbf{k}}$. So using crystallographic notation, we wrote the direction of the normal as $[h \ k \ l]$ (remember this is just to specify direction, we don't care about the magnitude). However, this was a special case. For a general set of crystal lattice vectors $\mathbf{a}$, $\mathbf{b}$ and $\mathbf{c}$, we need to use reciprocal lattice vectors to obtain the normal direction.

We know that we can get the normal to a plane if we can write down two vectors, $\mathbf{v}_1$ and $\mathbf{v}_2$, lying in the plane. Then the normal is just $\mathbf{v}_1 \times \mathbf{v}_2$. From the figure, we can see that the two suitable vectors are

$$\mathbf{v}_1 = \frac{\mathbf{b}}{k} - \frac{\mathbf{a}}{h} \quad \text{and} \quad \mathbf{v}_2 = \frac{\mathbf{c}}{l} - \frac{\mathbf{a}}{h}$$



So we need

$$\begin{aligned}\mathbf{v}_1 \times \mathbf{v}_2 &= \left(\frac{\mathbf{b}}{k} - \frac{\mathbf{a}}{h} \right) \times \left(\frac{\mathbf{c}}{l} - \frac{\mathbf{a}}{h} \right) \\ &= \frac{\mathbf{b} \times \mathbf{c}}{kl} - \frac{\mathbf{b} \times \mathbf{a}}{kh} - \frac{\mathbf{a} \times \mathbf{c}}{hl} + \mathbf{0}\end{aligned}$$

But we only care about the direction of the cross product, not the magnitude, so we can multiply by anything that makes the expression more simple:

$$hkl(\mathbf{v}_1 \times \mathbf{v}_2) = h\mathbf{b} \times \mathbf{c} + k\mathbf{c} \times \mathbf{a} + l\mathbf{a} \times \mathbf{b}$$

$$\frac{hkl}{\mathbf{a} \cdot (\mathbf{b} \times \mathbf{c})}(\mathbf{v}_1 \times \mathbf{v}_2) = h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^*$$

In other words, the direction of the normal to the plane $(h \ k \ l)$ is given by the vector $h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^*$. If we want the unit normal vector, we will write

$$\hat{\mathbf{n}} = \frac{h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^*}{|h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^*|}.$$

Example

2.3.4 The spacing of crystal planes

In a crystal there will be another plane, parallel to our plane (hkl) but containing the origin. What is the separation of these two planes? Well it is simply the distance of the origin from our plane. But we know that when a plane is defined by the standard equation, $\mathbf{r} \cdot \hat{\mathbf{n}} = c$, then $|c|$ is precisely this distance.

In our case, we have just found the expression for $\hat{\mathbf{n}}$. We also know three points lying in the plane: Namely, the ‘cut points’ $\mathbf{a}/h$, $\mathbf{b}/k$ and $\mathbf{c}/l$ (look again at Fig. 2.5). Any one of these points will suffice to work out c , e.g. substituting the first of them as $\mathbf{r}$ in the expression $c = \mathbf{r} \cdot \hat{\mathbf{n}}$ we find,

$$\begin{aligned} c = \frac{\mathbf{a}}{h} \cdot \hat{\mathbf{n}} &= \frac{\mathbf{a}}{h} \cdot \frac{h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^*}{|h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^*|} \\ &= \frac{1}{|h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^*|} \end{aligned}$$

So, for any general reciprocal lattice vector $\mathbf{v} = h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^*$, the direction of $\mathbf{v}$ is the normal to plane (hkl) , and $1/|\mathbf{v}|$ is the spacing between such planes.