

INTRODUCTION TO CONVENTIONAL TRANSMISSION ELECTRON MICROSCOPY

MARC DE GRAEF



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1

Basic crystallography

1.1 Introduction

In this chapter, we review the principles and basic tools of crystallography. A thorough understanding of crystallography is a prerequisite for anybody who wishes to learn transmission electron microscopy (TEM) and its applications to solid (mostly inorganic) materials. All diffraction techniques, whether they use x-rays, neutrons, or electrons, make extensive use of the concept of *reciprocal space* and, as we shall see repeatedly later on in this book, TEM is a unique tool for directly probing this space. Hence, it is important that the TEM user become as familiar with reciprocal space as with *direct* or *crystal space*.

This chapter will provide a sound mathematical footing for both direct and reciprocal space, mostly in the form of *non-Cartesian vector calculus*. Many textbooks on crystallography approach this type of vector calculus by explicitly stating the equations for, say, the length of a vector, in each of the seven crystal systems. While this is certainly correct, such tables of equations do not lend themselves to direct implementation in a computer program. In this book, we opt for a method which is independent of the crystal system and which can be implemented readily on a computer. We will introduce powerful tools for the computation of geometrical quantities (distances and angles) in both spaces and for a variety of coordinate transformations in and between those spaces. We will also discuss the *stereographic projection* (SP), an important tool for the analysis of electron diffraction patterns and crystal defects. The TEM user should be familiar with these basic tools.

Although many of these tools are available in commercial or public domain software packages, we will discuss them in sufficient detail so that the reader may also implement them in a new program. It is also useful to *understand* what the various menu-items in software programs really mean. We will minimize to the extent that it is possible the number of “black-box” routines used in this book. The reader may download ASCII files containing all of the routines discussed in this

book from the website. All of the algorithms are written in standard Fortran-90, and can easily be translated into C, Pascal, or any of the object-oriented languages (C++, Java, etc.). The user interface is kept simple, without on-screen graphics. Graphics output, if any, is produced in PostScript or TIFF format and can be viewed on-screen with an appropriate viewer or sent to a printer. The source code can be accessed at the Uniform Resource Locator (URL) <http://ctem.web.cmu.edu/>.

1.2 Direct space and lattice geometry

From a purely mathematical point of view, crystallography can be described as *vector calculus in a rectilinear, but not necessarily orthonormal (or even orthogonal) reference frame*. A discussion of crystallographic tools thus requires that we define basic vector operations in a non-Cartesian reference frame. Such operations are the *vector dot product*, the *vector cross product*, the computation of the length of a vector or the angle between two vectors, and so on.

1.2.1 Basis vectors and unit cells

A *crystal structure* is defined as a regular arrangement of atoms decorating a periodic, three-dimensional *lattice*. The lattice is defined as the set of points which is created by all *integer* linear combinations of three *basis vectors* **a**, **b**, and **c**. In other words, the lattice \mathcal{T} is the set of all vectors **t** of the form:

$$\mathbf{t} = u\mathbf{a} + v\mathbf{b} + w\mathbf{c},$$

with (u, v, w) being an arbitrary triplet of integers. We will often denote the basis vectors by the single symbol \mathbf{a}_i , where the subscript i takes on the values 1, 2, and 3. We will restrict ourselves to *right-handed* reference frames; i.e. the mixed product $(\mathbf{a} \times \mathbf{b}) \cdot \mathbf{c} > 0$. The *lattice vector* **t** can then be rewritten as

$$\mathbf{t} = \sum_{i=1}^3 u_i \mathbf{a}_i, \quad (1.1)$$

with $u_1 = u, u_2 = v$, and $u_3 = w$. This expression can be shortened even further by introducing the following notation convention, known as the *Einstein summation convention*: *If a subscript occurs twice in the same term of an equation, then a summation is implied over all values of this subscript and the corresponding summation sign need not be written*. In other words, since the subscript i occurs twice on the right-hand side of equation (1.1), we can drop the summation sign and simply write

$$\mathbf{t} = u_i \mathbf{a}_i. \quad (1.2)$$

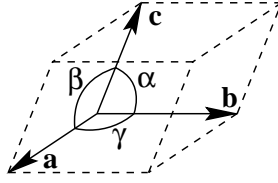


Fig. 1.1. Schematic representation of a general (triclinic or anorthic) unit cell.

The length of a vector is represented by the norm symbol $|\cdot|$; i.e. the length of the basis vector \mathbf{a}_i is $|\mathbf{a}_i|$ with $|\mathbf{a}_1| \equiv a$, $|\mathbf{a}_2| \equiv b$, and $|\mathbf{a}_3| \equiv c$. The angles between the basis vectors are represented by the Greek letters α , β , and γ , as indicated in Fig. 1.1. The six numbers $\{a, b, c, \alpha, \beta, \gamma\}$ are known as the *lattice parameters* of the unit cell.

The lattice parameters can be used to distinguish between the seven *crystal systems*:

$\{a, b, c, \alpha, \beta, \gamma\}$	$a \neq b \neq c; \alpha \neq \beta \neq \gamma$	triclinic or anorthic (a);
$\{a, b, c, \frac{\pi}{2}, \beta, \frac{\pi}{2}\}$	$a \neq b \neq c; \beta \neq \frac{\pi}{2}$	monoclinic (m);
$\{a, a, c, \frac{\pi}{2}, \frac{\pi}{2}, \frac{2\pi}{3}\}$	$a = b \neq c$	hexagonal (h);
$\{a, a, a, \alpha, \alpha, \alpha\}$	$a = b = c; \alpha \neq \frac{\pi}{2}$	rhombohedral (R);
$\{a, b, c, \frac{\pi}{2}, \frac{\pi}{2}, \frac{\pi}{2}\}$	$a \neq b \neq c$	orthorhombic (o);
$\{a, a, c, \frac{\pi}{2}, \frac{\pi}{2}, \frac{\pi}{2}\}$	$a = b \neq c$	tetragonal (t);
$\{a, a, a, \frac{\pi}{2}, \frac{\pi}{2}, \frac{\pi}{2}\}$	$a = b = c$	cubic (c).

It is a basic property of a lattice that all lattice sites are equivalent. In other words, any site can be selected as the *origin*. The seven crystal systems give rise to seven *primitive lattices*, since there is only one lattice site per unit cell. We can place additional lattice sites at the endpoints of so-called *centering vectors*; the possible centering vectors are:

$$\mathbf{A} = \left(0, \frac{1}{2}, \frac{1}{2}\right);$$

$$\mathbf{B} = \left(\frac{1}{2}, 0, \frac{1}{2}\right);$$

$$\mathbf{C} = \left(\frac{1}{2}, \frac{1}{2}, 0\right);$$

$$\mathbf{I} = \left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right).$$

A lattice with an extra site at the \mathbf{A} position is known as an *A-centered* lattice, and a site at the \mathbf{I} position gives rise to a *body-centered* or *I-centered* lattice. When the

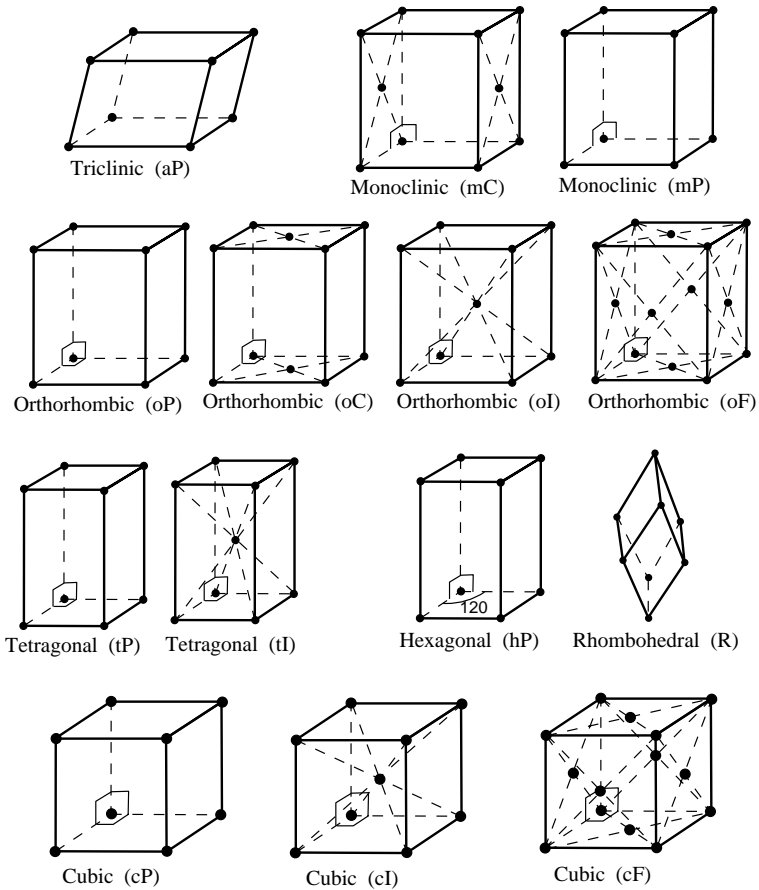


Fig. 1.2. The 14 Bravais lattices and their centering symbols.

three positions, **A**, **B**, and **C**, are simultaneously present as additional lattice sites, the lattice is *face centered* or *F-centered*.

When we combine these centering operations with each of the seven primitive unit cells, seven additional lattices are found. The 14 *Bravais lattices*, first derived by August Bravais in 1850 [Bra50], are shown in Fig. 1.2. They are commonly represented by two-letter symbols, the crystal system symbol followed by a centering symbol: *aP* (primitive anorthic), *mP* (primitive monoclinic), *mC* (C-centered monoclinic), *R* (primitive rhombohedral), *hP* (primitive hexagonal), *oP* (primitive orthorhombic), *oC* (C-centered orthorhombic), *oI* (body-centered orthorhombic), *oF* (face-centered orthorhombic), *tP* (primitive tetragonal), *tI* (body-centered tetragonal), *cP* (primitive cubic), *cI* (body-centered cubic), and *cF* (face-centered cubic). The choice of the lattice parameters of the Bravais lattices follows the conventions listed in the *International Tables for Crystallography, Volume A* [Hah96].

The vector \mathbf{t} in equation (1.1) represents a *direction* in the crystal lattice. It is usually represented by the symbol $[uvw]$ (square brackets, no commas between the components). Negative components are denoted by a minus sign above the corresponding component(s), e.g. $[\bar{u}v\bar{w}]$ for the vector with components $(-u, v, -w)$. Note that there is no agreement in the literature on how to pronounce the symbol $[\bar{u}v\bar{w}]$; some researchers will pronounce the *bar* before the number (i.e. bar u, v, bar w), while others will pronounce it following the number (i.e. u bar, v, w bar). Since one is referring to the negative of a number, and usually this is pronounced as “negative u”, or “minus u”, it makes sense to pronounce the bar *before* the number to which it applies.[†]

The position of an atom inside the unit cell is described by the position vector \mathbf{r} :

$$\mathbf{r} = x\mathbf{a} + y\mathbf{b} + z\mathbf{c} = \sum_{i=1}^3 r_i \mathbf{a}_i = r_i \mathbf{a}_i,$$

where we have again made use of the summation convention. The numbers (x, y, z) are real numbers between 0 and 1, and are known as *fractional coordinates*.

1.2.2 The dot product and the direct metric tensor

It is important that we have a method of computing distances between atoms and angles between interatomic bonds in the unit cell. Distances in a Cartesian reference frame are typically computed by means of Pythagoras’ Theorem: the distance D between two points P and Q with position vectors $\mathbf{p} = (p_1, p_2, p_3)$ and $\mathbf{q} = (q_1, q_2, q_3)$ is given by the length of the vector connecting the two points, or by the square root of the sum of the squares of the differences of the coordinates, i.e.

$$D = \sqrt{(p_1 - q_1)^2 + (p_2 - q_2)^2 + (p_3 - q_3)^2}.$$

In a non-Cartesian reference frame (and almost all crystallographic reference frames are non-Cartesian), this equation is no longer valid and it must be replaced by a more general expression that we shall now derive.

The dot product of two vectors \mathbf{p} and \mathbf{q} can be defined as the product of the lengths of \mathbf{p} and \mathbf{q} multiplied by the cosine of the angle θ between them, or

$\mathbf{p} \cdot \mathbf{q} \equiv |\mathbf{p}||\mathbf{q}| \cos \theta.$

The diagram shows two vectors, \mathbf{p} and \mathbf{q} , originating from the same point. Vector \mathbf{q} is horizontal, and vector \mathbf{p} is at an angle θ to it. A dashed line perpendicular to \mathbf{q} is dropped from the tip of \mathbf{p} , and a solid line segment along \mathbf{q} from the origin to the foot of the perpendicular is labeled $|\mathbf{p}|\cos\theta$.

(1.3)

[†] This is merely the author’s personal preference. The choice is really up to the reader.

This definition does not depend on a particular choice of reference frame, so it can be taken as a general definition of the dot product. The dot product can be interpreted as the projection of one vector onto a second vector, multiplied by the length of the second vector. If the two vectors are identical, we find (since $\theta = 0$)

$$\mathbf{p} \cdot \mathbf{p} = |\mathbf{p}|^2,$$

from which we derive

$$|\mathbf{p}| = \sqrt{\mathbf{p} \cdot \mathbf{p}}.$$

If the vector \mathbf{p} has components p_i with respect to the crystal basis vectors \mathbf{a}_i , we have[†]

$$|\mathbf{p}| = \sqrt{p_i \mathbf{a}_i \cdot p_j \mathbf{a}_j} = \sqrt{p_i (\mathbf{a}_i \cdot \mathbf{a}_j) p_j} \quad \left(= \sqrt{\sum_{i=1}^3 \sum_{j=1}^3 p_i (\mathbf{a}_i \cdot \mathbf{a}_j) p_j} \right).$$

We see that the *length* of a vector depends on all the dot products between the basis vectors (remember that there are two summations on the right-hand side of this equation!). The quantities $\mathbf{a}_i \cdot \mathbf{a}_j$ are of fundamental importance for crystallographic computations, and they are commonly denoted by the symbol

$$g_{ij} \equiv \mathbf{a}_i \cdot \mathbf{a}_j = |\mathbf{a}_i| |\mathbf{a}_j| \cos \theta_{ij}. \quad (1.4)$$

The nine numbers g_{ij} form a 3×3 matrix which is known as the *direct metric tensor*. From Fig. 1.1, we find that this matrix is given explicitly by

$$g_{ij} = \begin{bmatrix} \mathbf{a} \cdot \mathbf{a} & \mathbf{a} \cdot \mathbf{b} & \mathbf{a} \cdot \mathbf{c} \\ \mathbf{b} \cdot \mathbf{a} & \mathbf{b} \cdot \mathbf{b} & \mathbf{b} \cdot \mathbf{c} \\ \mathbf{c} \cdot \mathbf{a} & \mathbf{c} \cdot \mathbf{b} & \mathbf{c} \cdot \mathbf{c} \end{bmatrix} = \begin{bmatrix} a^2 & ab \cos \gamma & ac \cos \beta \\ ab \cos \gamma & b^2 & bc \cos \alpha \\ ac \cos \beta & bc \cos \alpha & c^2 \end{bmatrix}. \quad (1.5)$$

The matrix g_{ij} is *symmetric*[‡] since $g_{ij} = g_{ji}$. It has only six independent components corresponding to the six lattice parameters $\{a, b, c, \alpha, \beta, \gamma\}$. In other words, the metric tensor contains the same information as the set of lattice parameters, but in a form that allows direct computation of the dot product between two vectors. Explicit expressions for all seven metric tensors are listed in Appendix A1 on page 661.

Example 1.1 A tetragonal crystal has lattice parameters $a = \frac{1}{2} \text{ nm}$ and $c = 1 \text{ nm}$. Compute its metric tensor.

[†] The indices i and j are known as *dummy indices*; it does not really matter which symbols we use for such summation indices, as long as we use them consistently throughout the computation.

[‡] In this textbook, the first subscript of g_{ij} , or any other matrix, will always refer to the rows and the second subscript to the columns of g .

Answer: Substitution of these values into (1.5) results in

$$g_{ij} = \begin{bmatrix} \frac{1}{4} & 0 & 0 \\ 0 & \frac{1}{4} & 0 \\ 0 & 0 & 1 \end{bmatrix}.$$

Note that the units of the metric tensor elements are (nanometer)², but for brevity we usually drop them until the end of a computation.

The length of the vector \mathbf{p} can now be rewritten as

$$|\mathbf{p}| = \sqrt{p_i g_{ij} p_j}.$$

The argument of the square root contains a double summation over i and j . Since i is the row-index of the matrix g_{ij} , and since we can only multiply matrices that are *conformable*,[†] we find that the vector components p_i must be written in row form, while the components p_j must be written in column form, as follows:

$$|\mathbf{p}| = \sqrt{[p_1 \ p_2 \ p_3] \begin{bmatrix} a^2 & ab \cos \gamma & ac \cos \beta \\ ab \cos \gamma & b^2 & bc \cos \alpha \\ ac \cos \beta & bc \cos \alpha & c^2 \end{bmatrix} \begin{bmatrix} p_1 \\ p_2 \\ p_3 \end{bmatrix}}.$$

The dot product between two vectors \mathbf{p} and \mathbf{q} is given by

$$\boxed{\mathbf{p} \cdot \mathbf{q} = p_i \mathbf{a}_i \cdot q_j \mathbf{a}_j = p_i g_{ij} q_j,} \quad (1.6)$$

or explicitly

$$\mathbf{p} \cdot \mathbf{q} = [p_1 \ p_2 \ p_3] \begin{bmatrix} a^2 & ab \cos \gamma & ac \cos \beta \\ ab \cos \gamma & b^2 & bc \cos \alpha \\ ac \cos \beta & bc \cos \alpha & c^2 \end{bmatrix} \begin{bmatrix} q_1 \\ q_2 \\ q_3 \end{bmatrix}.$$

The angle θ between the two vectors is given by (from equation 1.3):

$$\boxed{\theta = \cos^{-1} \left(\frac{\mathbf{p} \cdot \mathbf{q}}{|\mathbf{p}| |\mathbf{q}|} \right) = \cos^{-1} \left(\frac{p_i g_{ij} q_j}{\sqrt{p_i g_{ij} p_j} \sqrt{q_i g_{ij} q_j}} \right).} \quad (1.7)$$

Example 1.2 For the tetragonal crystal in Example 1.1 on page 6, compute the distance between the points $(\frac{1}{2}, 0, \frac{1}{2})$ and $(\frac{1}{2}, \frac{1}{2}, 0)$.

Answer: The distance between two points is equal to the length of the vector connecting them, in this case $(\frac{1}{2} - \frac{1}{2}, 0 - \frac{1}{2}, \frac{1}{2} - 0) = (0, -\frac{1}{2}, \frac{1}{2})$. Using the tetragonal

[†] A matrix \mathcal{A} is said to be conformable with respect to \mathcal{B} if the number of columns in \mathcal{A} equals the number of rows in \mathcal{B} . Matrix multiplication is only defined for conformable matrices.

metric tensor derived previously, we find for the length of this vector:

$$\begin{aligned}
 |\mathbf{p}| &= \sqrt{\begin{bmatrix} 0 & \frac{-1}{2} & \frac{1}{2} \end{bmatrix} \begin{bmatrix} \frac{1}{4} & 0 & 0 \\ 0 & \frac{1}{4} & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 0 \\ \frac{-1}{2} \\ \frac{1}{2} \end{bmatrix}}; \\
 &= \sqrt{\begin{bmatrix} 0 & \frac{-1}{2} & \frac{1}{2} \end{bmatrix} \begin{bmatrix} 0 \\ \frac{-1}{8} \\ \frac{1}{2} \end{bmatrix}} = \frac{\sqrt{5}}{4} nm.
 \end{aligned}$$

Example 1.3 For the tetragonal unit cell of Example 1.1 on page 6, compute the dot product and the angle between the vectors $[120]$ and $[311]$.

Answer: The dot product is found from the expression for the metric tensor, as follows:

$$\mathbf{t}_{[120]} \cdot \mathbf{t}_{[311]} = [1 \ 2 \ 0] \begin{bmatrix} \frac{1}{4} & 0 & 0 \\ 0 & \frac{1}{4} & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 3 \\ 1 \\ 1 \end{bmatrix} = [1 \ 2 \ 0] \begin{bmatrix} \frac{3}{4} \\ \frac{1}{4} \\ 1 \end{bmatrix} = \frac{5}{4} nm^2.$$

The angle is found by dividing the dot product by the lengths of the vectors, $|[120]|^2 = \frac{5}{4} nm^2$ and $|[311]|^2 = \frac{14}{4} nm^2$, from which we find

$$\cos \theta = \frac{\frac{5}{4}}{\sqrt{\frac{14}{4}} \sqrt{\frac{5}{4}}} = \frac{5}{\sqrt{70}} \rightarrow \theta = 53.30^\circ.$$

Example 1.4 The angle between two direct space vectors can be computed in a single operation, instead of using the three individual dot products described in the previous example. Derive a procedure for computing the angle θ based on a 2×3 matrix containing the two vectors \mathbf{p} and \mathbf{q} .

Answer: Consider the following formal relation:

$$\begin{pmatrix} \mathbf{p} \\ \mathbf{q} \end{pmatrix} \cdot (\mathbf{p} \ \mathbf{q}) = \begin{pmatrix} \mathbf{p} \cdot \mathbf{p} & \mathbf{p} \cdot \mathbf{q} \\ \mathbf{q} \cdot \mathbf{p} & \mathbf{q} \cdot \mathbf{q} \end{pmatrix}.$$

The resulting 2×2 matrix contains all three dot products needed for the computation of the angle θ , and only one set of matrix multiplications is needed. We can apply this short cut to the previous example:

$$\begin{pmatrix} 1 & 2 & 0 \\ 3 & 1 & 1 \end{pmatrix} \begin{pmatrix} \frac{1}{4} & 0 & 0 \\ 0 & \frac{1}{4} & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 3 \\ 2 & 1 \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} \frac{5}{4} & \frac{5}{4} \\ \frac{5}{4} & \frac{14}{4} \end{pmatrix},$$

from which we find the same angle of $\theta = 53.30^\circ$.

Note that these equations are valid in every rectilinear coordinate frame[†] and, therefore, in every crystal system. Explicit expressions for distances and angles in the seven reference frames are listed in Appendix A1 on pages 663–664. For a Cartesian, orthonormal reference frame, the metric tensor reduces to the identity matrix. Indeed, the Cartesian basis vectors \mathbf{e}_i have unit length and are orthogonal to each other; therefore, the metric tensor reduces to

$$g_{ij} = \begin{bmatrix} \mathbf{e}_1 \cdot \mathbf{e}_1 & \mathbf{e}_1 \cdot \mathbf{e}_2 & \mathbf{e}_1 \cdot \mathbf{e}_3 \\ \mathbf{e}_2 \cdot \mathbf{e}_1 & \mathbf{e}_2 \cdot \mathbf{e}_2 & \mathbf{e}_2 \cdot \mathbf{e}_3 \\ \mathbf{e}_3 \cdot \mathbf{e}_1 & \mathbf{e}_3 \cdot \mathbf{e}_2 & \mathbf{e}_3 \cdot \mathbf{e}_3 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \equiv \delta_{ij}, \quad (1.8)$$

where we have introduced the *Kronecker delta* δ_{ij} , which is equal to 1 for $i = j$ and 0 for $i \neq j$. Substitution into equation (1.6) results in

$$\mathbf{p} \cdot \mathbf{q} = p_i \delta_{ij} q_j = p_i q_i = p_1 q_1 + p_2 q_2 + p_3 q_3,$$

which is the standard expression for the dot product between two vectors in a Cartesian reference frame. We will postpone until Section 1.9 a discussion of how to implement the metric tensor formalism on a computer.

1.3 Definition of reciprocal space

In the previous section, we have described how we can compute distances between atoms in a crystal and angles between the bonds connecting those atoms. In Chapter 2, we will see that *diffraction* of electrons is described by the *Bragg equation*, which relates the diffraction angle to the electron wavelength and the spacing between crystal planes. We must, therefore, devise a tool that will enable us to compute this spacing between successive lattice planes in an arbitrary crystal lattice. We would like to have a method similar to that described in the previous section, ideally one with equations identical in form to those for the distance between atoms or the dot product between direction vectors. It turns out that such a tool exists and we will introduce the *reciprocal metric tensor* in the following subsections.

1.3.1 Planes and Miller indices

The description of crystal planes has a long history going all the way back to *René-Juste Haüy* [Häu84] who formulated the *Second Law of Crystal Habit*, also known as the law of simple rational intercepts. This law prompted *Miller* to devise a system to label crystal planes, based on their intercepts with the crystallographic reference axes. Although the so-called *Miller indices* were used by several crystallographers before Miller, they are attributed to him because he used them extensively in his book and teachings [Mil39] and because he developed the familiar *hkl* notation.

[†] They are also valid for curvilinear coordinate frames, but we will not make much use of such reference frames in this book.

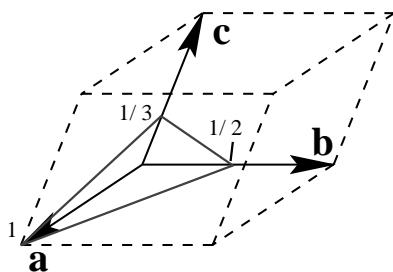


Fig. 1.3. Illustration of the determination of the Miller indices of a plane.

The Miller indices of a plane in an arbitrary crystal system are obtained in the following way.

- (i) If the plane goes through the origin, then displace it so that it no longer contains the origin.
- (ii) Determine the intercepts of the plane with the three basis vectors. Call those intercepts s_1 , s_2 , and s_3 . The intercepts must be measured in units of the basis vector length. For the plane shown in Fig. 1.3, these values are $s_1 = 1$, $s_2 = \frac{1}{2}$, and $s_3 = \frac{1}{3}$. If a plane is parallel to one or more of the basis vectors, then the corresponding intercept value(s) must be taken as ∞ .
- (iii) Invert all three intercepts. For the plane in the figure we find $\frac{1}{s_1} = 1$, $\frac{1}{s_2} = 2$, and $\frac{1}{s_3} = 3$. If one of the intercepts is ∞ , then the corresponding number is zero.
- (iv) Reduce the three numbers to the smallest possible integers (relative primes). (This is not necessary for the example above.)
- (v) Write the three numbers surrounded by round brackets, i.e. (123). This triplet of numbers forms the *Miller indices* of the plane.

In general, the Miller indices of a plane are denoted by the symbol (hkl) . As for directions, negative indices are indicated by a *bar* or minus sign written above the corresponding index, e.g. $(\bar{1}2\bar{3})$. Although Miller indices were defined as relative primes, we will see later on that it is often necessary to consider planes of the type $(nh\ nk\ nl)$, where n is a non-zero integer. All planes of this type are parallel to the plane (hkl) , but for diffraction purposes they are not the same as the plane (hkl) . For instance, the plane (111) is parallel to the plane (222), but the two planes behave differently in a diffraction experiment.

1.3.2 The reciprocal basis vectors

It is tempting to interpret the triplet of Miller indices (hkl) as the components of a vector. A quick inspection of the orientation of the vector $\mathbf{n} = h\mathbf{a} + k\mathbf{b} + l\mathbf{c}$ with respect to the plane (hkl) in an arbitrary crystal system shows that, except

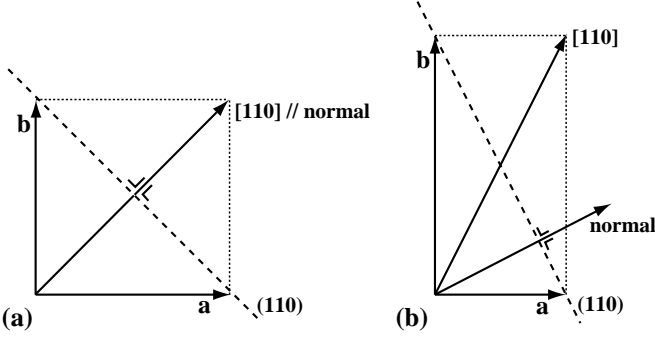


Fig. 1.4. (a) In a cubic (square) lattice, a direction vector $[110]$ is normal to the plane with Miller indices (110) ; this is no longer the case for a non-cubic system, as shown in the rectangular cell (b).

in special cases, there is no fixed relation between the two (see Fig. 1.4). In other words, when the Miller indices are interpreted as the components of a vector with respect to the direct basis vectors \mathbf{a}_i , we do not find a useful relationship between this vector and the plane (hkl) . We must then ask the question: can we find three new basis vectors \mathbf{a}^* , \mathbf{b}^* , and \mathbf{c}^* , related to the direct basis vectors \mathbf{a}_i , such that the vector $\mathbf{g} = h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^*$ conveys meaningful information about the plane (hkl) ? It turns out that such a triplet of basis vectors exists, and they are known as the *reciprocal basis vectors*. We will distinguish them from the direct basis vectors by means of an asterisk, \mathbf{a}_j^* .

The reciprocal basis vectors can be derived from the following definition:

$$\boxed{\mathbf{a}_i \cdot \mathbf{a}_j^* \equiv \delta_{ij}}, \quad (1.9)$$

where δ_{ij} is the Kronecker delta introduced in equation (1.8). This expression fully defines the reciprocal basis vectors: it states that the vector \mathbf{a}^* must be perpendicular to both \mathbf{b} and \mathbf{c} ($\mathbf{a}^* \cdot \mathbf{b} = \mathbf{a}^* \cdot \mathbf{c} = 0$), and that $\mathbf{a}^* \cdot \mathbf{a} = 1$. The first condition is satisfied if \mathbf{a}^* is parallel to the cross product between \mathbf{b} and \mathbf{c} :

$$\mathbf{a}^* = K(\mathbf{b} \times \mathbf{c}),$$

where K is a constant. The second condition leads to the value of K :

$$\mathbf{a} \cdot \mathbf{a}^* = K\mathbf{a} \cdot (\mathbf{b} \times \mathbf{c}) = 1,$$

from which we find

$$K = \frac{1}{\mathbf{a} \cdot (\mathbf{b} \times \mathbf{c})} \equiv \frac{1}{\Omega},$$

where Ω is the volume of the unit cell formed by the vectors \mathbf{a}_i .

A similar procedure for the remaining two reciprocal basis vectors then leads to the following expressions:

$$\left. \begin{aligned} \mathbf{a}^* &= \frac{\mathbf{b} \times \mathbf{c}}{\mathbf{a} \cdot (\mathbf{b} \times \mathbf{c})}; \\ \mathbf{b}^* &= \frac{\mathbf{c} \times \mathbf{a}}{\mathbf{a} \cdot (\mathbf{b} \times \mathbf{c})}; \\ \mathbf{c}^* &= \frac{\mathbf{a} \times \mathbf{b}}{\mathbf{a} \cdot (\mathbf{b} \times \mathbf{c})}. \end{aligned} \right\} \quad (1.10)$$

We define the *reciprocal lattice* \mathcal{T}^* as the set of end-points of the vectors of the type

$$\mathbf{g} = h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^* = \sum_{i=1}^3 g_i \mathbf{a}_i^* = g_i \mathbf{a}_i^*,$$

where (h, k, l) are integer triplets. This new lattice is also known as the *dual lattice*, but in the diffraction world we prefer the name *reciprocal lattice*. We will now investigate the relation between the reciprocal lattice vectors \mathbf{g} and the planes with Miller indices (hkl) .

We will look for all the direct space vectors \mathbf{r} with components $r_i = (x, y, z)$ that are perpendicular to the vector \mathbf{g} . We already know that two vectors are perpendicular to each other if their dot product vanishes. In this case we find:

$$0 = \mathbf{r} \cdot \mathbf{g} = (r_i \mathbf{a}_i) \cdot (g_j \mathbf{a}_j^*) = r_i (\mathbf{a}_i \cdot \mathbf{a}_j^*) g_j.$$

We also know from equation (1.9) that the last dot product is equal to δ_{ij} , so

$$\mathbf{r} \cdot \mathbf{g} = r_i \delta_{ij} g_j = r_i g_i = r_1 g_1 + r_2 g_2 + r_3 g_3 = hx + ky + lz = 0. \quad (1.11)$$

The components of the vector \mathbf{r} must satisfy the relation $hx + ky + lz = 0$ if \mathbf{r} is to be perpendicular to \mathbf{g} . This relation represents the equation of a plane through the origin of the direct crystal lattice. If a plane intersects the basis vectors \mathbf{a}_i at intercepts s_i , then the equation of that plane is given by [Spi68]

$$\frac{x}{s_1} + \frac{y}{s_2} + \frac{z}{s_3} = 1, \quad (1.12)$$

where (x, y, z) is an arbitrary point in the plane. The right-hand side of this equation takes on different values when we translate the plane along its normal, and, in particular, is equal to zero when the plane goes through the origin. Comparing

$$hx + ky + lz = 0$$

with

$$\frac{x}{s_1} + \frac{y}{s_2} + \frac{z}{s_3} = 0,$$

we find that the integers h , k , and l are reciprocals of the intercepts of a plane with the direct lattice basis vectors. This is exactly the definition of the *Miller indices* of a plane! We thus find the fundamental result:

The reciprocal lattice vector \mathbf{g} , with components (h, k, l) , is perpendicular to the plane with Miller indices (hkl) .

For this reason, a reciprocal lattice vector is often denoted with the Miller indices as subscripts, e.g. \mathbf{g}_{hkl} .

Since the vector $\mathbf{g} = g_i \mathbf{a}_i^*$ is perpendicular to the plane with Miller indices $g_i = (hkl)$, the unit normal to this plane is given by

$$\mathbf{n} = \frac{\mathbf{g}_{hkl}}{|\mathbf{g}_{hkl}|}.$$

The perpendicular distance from the origin to the plane intersecting the direct basis vectors at the points $\frac{1}{h}$, $\frac{1}{k}$, and $\frac{1}{l}$ is given by the projection of any vector \mathbf{t} ending in the plane onto the plane normal \mathbf{n} (see Fig. 1.5). This distance is also, by definition, the *interplanar spacing* d_{hkl} . Thus,

$$\mathbf{t} \cdot \mathbf{n} = \mathbf{t} \cdot \frac{\mathbf{g}_{hkl}}{|\mathbf{g}_{hkl}|} \equiv d_{hkl}.$$

We can arbitrarily select $\mathbf{t} = \frac{\mathbf{a}}{h}$, which leads to

$$\mathbf{t} \cdot \mathbf{g}_{hkl} = \frac{\mathbf{a}}{h} \cdot (h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^*) = \frac{\mathbf{a}}{h} \cdot h\mathbf{a}^* = 1 = d_{hkl}|\mathbf{g}_{hkl}|,$$

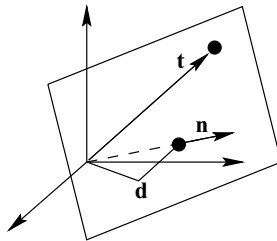


Fig. 1.5. The distance of a plane to the origin equals the projection of any vector \mathbf{t} ending in this plane onto the unit plane normal \mathbf{n} .

from which we find

$$|\mathbf{g}_{hkl}| = \frac{1}{d_{hkl}}. \quad (1.13)$$

The length of a reciprocal lattice vector is equal to the inverse of the spacing between the corresponding lattice planes.

We thus find that every vector \mathbf{g}_{hkl} of the reciprocal lattice is parallel to the normal to the set of planes with Miller indices (hkl) , and the length of \mathbf{g}_{hkl} (i.e. the distance from the point (h, k, l) to the origin of the reciprocal lattice) is equal to the inverse of the spacing between consecutive lattice planes. At this point, it is useful to introduce methods for lattice calculations in the reciprocal lattice; we will see that the metric tensor formalism introduced in Section 1.2.2 can also be applied to the reciprocal lattice.

1.3.3 Lattice geometry in reciprocal space

We know that the length of a vector is given by the square root of the dot product of this vector with itself. Thus, the length of \mathbf{g} is given by

$$\frac{1}{d_{hkl}} = |\mathbf{g}| = \sqrt{\mathbf{g} \cdot \mathbf{g}} = \sqrt{(g_i \mathbf{a}_i^*) \cdot (g_j \mathbf{a}_j^*)} = \sqrt{g_i (\mathbf{a}_i^* \cdot \mathbf{a}_j^*) g_j}.$$

Again we find that the general dot product involves knowledge of the dot products of the basis vectors, in this case the reciprocal basis vectors. We introduce the *reciprocal metric tensor*:

$$g_{ij}^* \equiv \mathbf{a}_i^* \cdot \mathbf{a}_j^*. \quad (1.14)$$

Explicitly, the reciprocal metric tensor is given by:

$$\begin{aligned} g^* &= \begin{bmatrix} \mathbf{a}^* \cdot \mathbf{a}^* & \mathbf{a}^* \cdot \mathbf{b}^* & \mathbf{a}^* \cdot \mathbf{c}^* \\ \mathbf{b}^* \cdot \mathbf{a}^* & \mathbf{b}^* \cdot \mathbf{b}^* & \mathbf{b}^* \cdot \mathbf{c}^* \\ \mathbf{c}^* \cdot \mathbf{a}^* & \mathbf{c}^* \cdot \mathbf{b}^* & \mathbf{c}^* \cdot \mathbf{c}^* \end{bmatrix}; \\ &= \begin{bmatrix} a^{*2} & a^* b^* \cos \gamma^* & a^* c^* \cos \beta^* \\ b^* a^* \cos \gamma^* & b^{*2} & b^* c^* \cos \alpha^* \\ c^* a^* \cos \beta^* & c^* b^* \cos \alpha^* & c^{*2} \end{bmatrix}, \end{aligned} \quad (1.15)$$

where $\{a^*, b^*, c^*, \alpha^*, \beta^*, \gamma^*\}$ are the reciprocal lattice parameters. Explicit expressions for all seven reciprocal metric tensors are given in Appendix A1 on page 662.

In Section 1.3.4, we will develop an easy way to compute the reciprocal basis vectors and lattice parameters; for now the explicit equations in the appendix are sufficient.

Example 1.5 Compute the reciprocal metric tensor for a tetragonal crystal with lattice parameters $a = \frac{1}{2}$ and $c = 1$.

Answer: Substitution of the lattice parameters into the expression for the tetragonal reciprocal metric tensor in Appendix A1 yields

$$\mathbf{g}_{\text{tetragonal}}^* = \begin{bmatrix} 4 & 0 & 0 \\ 0 & 4 & 0 \\ 0 & 0 & 1 \end{bmatrix}.$$

We can now rewrite the length of the reciprocal lattice vector \mathbf{g} as

$$\frac{1}{d_{hkl}} = |\mathbf{g}| = \sqrt{\mathbf{g} \cdot \mathbf{g}} = \sqrt{g_i g_{ij}^* g_j}. \quad (1.16)$$

The angle θ between two reciprocal lattice vectors \mathbf{f} and \mathbf{g} is given by the standard relation (equation 1.7):

$$\theta = \cos^{-1} \left(\frac{f_i g_{ij}^* g_j}{\sqrt{f_i g_{ij}^* f_j} \sqrt{g_i g_{ij}^* g_j}} \right). \quad (1.17)$$

Example 1.6 Compute the angle between the (120) and (311) plane normals for the tetragonal crystal of Example 1.5.

Answer: Substitution of the vector components and the reciprocal metric tensor into the expression for the angle results in

$$\begin{aligned} \cos \theta &= \frac{[1\ 2\ 0] \begin{bmatrix} 4 & 0 & 0 \\ 0 & 4 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 3 \\ 1 \\ 1 \end{bmatrix}}{\sqrt{[1\ 2\ 0] \begin{bmatrix} 4 & 0 & 0 \\ 0 & 4 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 \\ 2 \\ 0 \end{bmatrix}} \sqrt{[3\ 1\ 1] \begin{bmatrix} 4 & 0 & 0 \\ 0 & 4 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 3 \\ 1 \\ 1 \end{bmatrix}}}, \\ &= \frac{20}{\sqrt{20 \times 41}} = 0.69843, \\ &\rightarrow \theta = 45.7^\circ. \end{aligned}$$

Example 1.7 *Redo the computation of the previous example using the shorthand notation introduced in Example 1.4.*

Answer: *The matrix product is given by*

$$\begin{pmatrix} 1 & 2 & 0 \\ 3 & 1 & 1 \end{pmatrix} \begin{pmatrix} 4 & 0 & 0 \\ 0 & 4 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 3 \\ 2 & 1 \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} 20 & 20 \\ 20 & 41 \end{pmatrix},$$

from which we find the same angle of $\theta = 45.7^\circ$.

Note that we have indeed managed to create a computational tool that is formally identical to that used for distances and angles in direct space. This should come as no surprise, since the reciprocal basis vectors are just another set of basis vectors, and the equations for direct space must be valid for *any* non-Cartesian reference frame. The particular choice for the reciprocal basis vectors (see equation 1.9) guarantees that they are useful for the description of lattice planes. In the next section, we will derive relations between the direct and reciprocal lattices.

1.3.4 Relations between direct space and reciprocal space

We know that a vector is a mathematical object that exists independently of the reference frame. This means that every vector defined in the direct lattice must also have components with respect to the reciprocal basis vectors and vice versa. In this section, we will devise a tool that will permit us to transform vector quantities back and forth between direct and reciprocal space.

Consider the vector \mathbf{p} :

$$\mathbf{p} = p_i \mathbf{a}_i = p_j^* \mathbf{a}_j^*,$$

where p_j^* are the reciprocal space components of \mathbf{p} . Multiplying both sides by the direct basis vector \mathbf{a}_m , we have

$$\left. \begin{aligned} p_i \mathbf{a}_i \cdot \mathbf{a}_m &= p_j^* \mathbf{a}_j^* \cdot \mathbf{a}_m, \\ p_i g_{im} &= p_j^* \delta_{jm} = p_m^*, \end{aligned} \right\} \quad (1.18)$$

or

$$p_m^* = p_i g_{im}. \quad (1.19)$$

It is easily shown that the inverse relation is given by

$$p_i = p_m^* g_{mi}^*. \quad (1.20)$$

We thus find that *post-multiplication by the metric tensor* transforms vector components from direct space to reciprocal space, and post-multiplication by the reciprocal

metric tensor transforms vector components from reciprocal to direct space. These relations are useful because they permit us to determine the components of a direction vector $\mathbf{t}_{[uvw]}$ with respect to the reciprocal basis vectors, or the components of a plane normal \mathbf{g}_{hkl} with respect to the direct basis vectors.

Example 1.8 *For the tetragonal unit cell of Example 1.1 on page 6, write down the reciprocal components of the lattice vector [114].*

Answer: *This transformation is accomplished by post-multiplication by the direct metric tensor:*

$$t_{[114]}^* = [1 \ 1 \ 4] \begin{bmatrix} \frac{1}{4} & 0 & 0 \\ 0 & \frac{1}{4} & 0 \\ 0 & 0 & 1 \end{bmatrix} = \left[\frac{1}{4} \ \frac{1}{4} \ 4 \right].$$

In other words, the [114] direction is perpendicular to the (1 1 16) plane.

Now we have all the tools we need to express the reciprocal basis vectors in terms of the direct basis vectors. Consider again the vector \mathbf{p} :

$$\mathbf{p} = p_i \mathbf{a}_i.$$

If we replace p_i by $p_m^* g_{mi}^*$, then we have

$$\mathbf{p} = p_m^* g_{mi}^* \mathbf{a}_i = p_m^* \mathbf{a}_m^*,$$

from which we find

$$\mathbf{a}_m^* = g_{mi}^* \mathbf{a}_i, \quad (1.21)$$

and the inverse relation

$$\mathbf{a}_m = g_{mi} \mathbf{a}_i^*. \quad (1.22)$$

In other words, the rows of the metric tensor contain the components of the direct basis vectors in terms of the reciprocal basis vectors, whereas the rows of the reciprocal metric tensor contain the components of the reciprocal basis vectors with respect to the direct basis vectors.

Finally, from equation (1.22) we find after multiplication by the vector \mathbf{a}_k^* :

$$\left. \begin{aligned} \mathbf{a}_m \cdot \mathbf{a}_k^* &= g_{mi} \mathbf{a}_i^* \cdot \mathbf{a}_k^*, \\ \delta_{mk} &= g_{mi} g_{ik}^*. \end{aligned} \right\} \quad (1.23)$$

In other words, the matrices representing the direct and reciprocal metric tensors are each other's inverse. This leads to a simple procedure to determine the reciprocal

basis vectors of a crystal:

- (i) compute the direct metric tensor;
- (ii) invert it to find the reciprocal metric tensor;
- (iii) apply equation (1.21) to find the reciprocal basis vectors.

Example 1.9 *For the tetragonal unit cell of the previous example, write down the explicit expressions for the reciprocal basis vectors. From these expressions, derive the reciprocal lattice parameters.*

Answer: *The components of the reciprocal basis vectors are given by the rows of the reciprocal metric tensor; and thus*

$$\mathbf{a}_1^* = 4\mathbf{a}_1;$$

$$\mathbf{a}_2^* = 4\mathbf{a}_2;$$

$$\mathbf{a}_3^* = \mathbf{a}_3.$$

The reciprocal lattice parameters are now easily found from the lengths of the basis vectors: $a^ = |\mathbf{a}_1^*| = |\mathbf{a}_2^*| = 4|\mathbf{a}_1| = 4 \times \frac{1}{2} = 2 \text{ nm}^{-1}$, and $c^* = |\mathbf{a}_3^*| = |\mathbf{a}_3| = 1 \text{ nm}^{-1}$. The angles between the reciprocal basis vectors are all 90° .*

1.3.5 The non-Cartesian vector cross product

The attentive reader may have noticed that we have made use of the *vector cross product* in the definition of the reciprocal lattice vectors, without considering how the cross product is defined in a non-Cartesian reference frame. In this section, we will generalize the cross product to crystallographic reference frames.

Consider the two real-space vectors $\mathbf{p} = p_1\mathbf{a} + p_2\mathbf{b} + p_3\mathbf{c}$ and $\mathbf{q} = q_1\mathbf{a} + q_2\mathbf{b} + q_3\mathbf{c}$. The cross product between them is defined as

$$\mathbf{p} \times \mathbf{q} \equiv \sin \theta |\mathbf{p}| |\mathbf{q}| \mathbf{z},$$

(1.24)

where θ is the angle between \mathbf{p} and \mathbf{q} , and \mathbf{z} is a unit vector perpendicular to both \mathbf{p} and \mathbf{q} . The length of the cross product vector is equal to the area of the parallelogram enclosed by the vectors \mathbf{p} and \mathbf{q} . It is straightforward to compute the components

of the cross product:

$$\begin{aligned}\mathbf{p} \times \mathbf{q} &= p_1 q_1 \mathbf{a} \times \mathbf{a} + p_1 q_2 \mathbf{a} \times \mathbf{b} + p_1 q_3 \mathbf{a} \times \mathbf{c} \\ &\quad + p_2 q_1 \mathbf{b} \times \mathbf{a} + p_2 q_2 \mathbf{b} \times \mathbf{b} + p_2 q_3 \mathbf{b} \times \mathbf{c} \\ &\quad + p_3 q_1 \mathbf{c} \times \mathbf{a} + p_3 q_2 \mathbf{c} \times \mathbf{b} + p_3 q_3 \mathbf{c} \times \mathbf{c}.\end{aligned}$$

Since the cross product of a vector with itself vanishes, and $\mathbf{a} \times \mathbf{b} = -\mathbf{b} \times \mathbf{a}$, we can rewrite this equation as:

$$\begin{aligned}\mathbf{p} \times \mathbf{q} &= (p_1 q_2 - p_2 q_1) \mathbf{a} \times \mathbf{b} + (p_2 q_3 - p_3 q_2) \mathbf{b} \times \mathbf{c} + (p_3 q_1 - p_1 q_3) \mathbf{c} \times \mathbf{a} \\ &= \Omega[(p_2 q_3 - p_3 q_2) \mathbf{a}^* + (p_3 q_1 - p_1 q_3) \mathbf{b}^* + (p_1 q_2 - p_2 q_1) \mathbf{c}^*], \quad (1.25)\end{aligned}$$

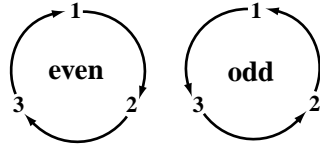
where we have used the definition of the reciprocal basis vectors (equation 1.10). We thus find that the vector cross product between two vectors in direct space is described by a vector expressed in the reciprocal reference frame! This is to be expected since the vector cross product results in a vector perpendicular to the plane formed by the two initial vectors, and we know that the reciprocal reference frame deals with such normals to planes.

In a Cartesian reference frame, the reciprocal basis vectors are identical to the direct basis vectors $\mathbf{e}_i = \mathbf{e}_i^*$ (this follows from equation (1.21) and from the fact that the direct metric tensor is the identity matrix), and the unit cell volume is equal to 1, so the expression for the cross product reduces to the familiar expression:

$$\mathbf{p} \times \mathbf{q} = (p_2 q_3 - p_3 q_2) \mathbf{e}_1 + (p_3 q_1 - p_1 q_3) \mathbf{e}_2 + (p_1 q_2 - p_2 q_1) \mathbf{e}_3.$$

We introduce a new symbol, the *normalized permutation symbol* e_{ijk} . This symbol is defined as follows:

$$e_{ijk} = \begin{cases} +1 & \text{even permutations of 123,} \\ -1 & \text{odd permutations of 123,} \\ 0 & \text{all other cases.} \end{cases}$$



The even permutations of the indices ijk are 123, 231, and 312; the odd permutations are 321, 213, and 132. For all other combinations, the permutation symbol vanishes. The sketch on the right shows an easy way to remember the combinations. We can now rewrite equation (1.25) as

$$\boxed{\mathbf{p} \times \mathbf{q} = \Omega e_{ijk} p_i q_j \mathbf{a}_k^*} \quad (1.26)$$

Note that this is equivalent to the more conventional determinantal notation for the cross product:

$$\mathbf{p} \times \mathbf{q} = \Omega \begin{vmatrix} \mathbf{a}_1^* & \mathbf{a}_2^* & \mathbf{a}_3^* \\ p_1 & p_2 & p_3 \\ q_1 & q_2 & q_3 \end{vmatrix} \left(= \begin{vmatrix} \mathbf{e}_1 & \mathbf{e}_2 & \mathbf{e}_3 \\ p_1 & p_2 & p_3 \\ q_1 & q_2 & q_3 \end{vmatrix} \text{Cartesian} \right).$$

Using equation (1.21), we also find

$$\boxed{\mathbf{p} \times \mathbf{q} = \Omega e_{ijk} p_i q_j g_{km}^* \mathbf{a}_m.} \quad (1.27)$$

The general definition of the cross product can be used in a variety of situations. A few examples are as follows.

- (i) We can rewrite the definition of the reciprocal basis vectors (1.10) as a single equation, using the permutation symbol:

$$\mathbf{a}_i^* = \frac{1}{2\Omega} e_{ijk} (\mathbf{a}_j \times \mathbf{a}_k), \quad (1.28)$$

where a summation over j and k is implied. From this relation, we can also derive equation (1.21).

- (ii) The volume Ω of the unit cell is given by the mixed product of the three basis vectors:[†]

$$\begin{aligned} \mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3) &= \Omega \mathbf{a}_1 \cdot [e_{ijk} \mathbf{a}_{2,i} \mathbf{a}_{3,j} g_{km}^* \mathbf{a}_m], \\ &= \Omega e_{ijk} \delta_{2i} \delta_{3j} g_{km}^* \mathbf{a}_1 \cdot \mathbf{a}_m, \\ &= \Omega e_{23k} g_{km}^* g_{m1}, \\ &= \Omega e_{231} g_{1m}^* g_{m1}, \\ &= \Omega \delta_{11}, \\ &= \Omega. \end{aligned}$$

Example 1.10 Determine the cross product of the vectors $[110]$ and $[111]$ in the tetragonal lattice of Example 1.1 on page 6.

Answer: From the general expression for the cross product we find

$$\begin{aligned} \mathbf{t}_{[110]} \times \mathbf{t}_{[111]} &= \Omega e_{ijk} \mathbf{t}_{[110],i} \mathbf{t}_{[111],j} \mathbf{a}_k^*, \\ &= \frac{1}{4} [(1 \times 1 - 0 \times 1) \mathbf{a}_1^* + (0 \times 1 - 1 \times 1) \mathbf{a}_2^* + (1 \times 1 - 1 \times 1) \mathbf{a}_3^*], \\ &= \frac{1}{4} (\mathbf{a}_1^* - \mathbf{a}_2^*). \end{aligned}$$

Using the solution for Example 1.9 on page 18, this is also equal to $\mathbf{a}_1 - \mathbf{a}_2$ or the direction vector $[1\bar{1}0]$.

[†] $\mathbf{a}_{i,j}$ is the j th component of the basis vector \mathbf{a}_i , expressed in the direct reference frame \mathbf{a}_i .