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The Use of a Redundant Axis in Defining the Basis of a Lattice

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The description of n-dimensional space by a basis of $(n+1)$ vectors, $\mathbf{a}_i$ $(i=1, \ldots, n+1)$, is discussed, with particular reference to the Miller–Bravais system of indexing hexagonal crystals. It is shown that if a hyperplane with normal $\mathbf{h}$ makes intercepts h_i^{-1} on the $\mathbf{a}_i$ and a vector $\mathbf{u}$ has components u_i relative to the $\mathbf{a}_i$, then $\mathbf{h} \cdot \mathbf{u} = \sum h_i u_i$ without any further restrictions on the h_i or u_i. Furthermore, it is possible to find a basis $\mathbf{a}_i^\dagger (i=1, \ldots, n+1)$ for reciprocal space such that $\mathbf{h} = \sum h_i \mathbf{a}_i^\dagger$ is always true and indeed there are n degrees of freedom available for choosing such a basis. Criteria which may lead to a unique choice of $\mathbf{a}_i^\dagger$ are discussed.

1. Introduction

Hexagonal crystals are usually described by means of the so-called Miller–Bravais 4-index system, since the 4 axes [${}_H\mathbf{a}_i$, $i=1,2,3$, and $\mathbf{c}$ in Fig. 1(*a*)] provide a symmetrical basis for the hexagonal lattice and it is possible to find a similarly symmetric basis [${}_H\mathbf{a}_i^\dagger$, $i=1,2,3$, and $\mathbf{c}^\dagger$ in Fig. 1(*b*)] to describe the reciprocal lattice. Although these bases are, of course, not reciprocal to one another (see *e.g.* Nicholas, 1970), they have the properties that:

(*a*) if the indices of a plane (*hkil*) are defined as the reciprocals of its intercepts on ${}_H\mathbf{a}_i$ and $\mathbf{c}$, then

$$h+k+i=0\,, \tag{1}$$

and the normal to the plane is given by

$$\mathbf{h}=h\,{}_H\mathbf{a}_1^\dagger+k\,{}_H\mathbf{a}_2^\dagger+i\,{}_H\mathbf{a}_3^\dagger+l\mathbf{c}^\dagger, \tag{2}$$

where the magnitude of $\mathbf{h}$ is equal to the reciprocal of the distance of the plane from the origin; and

(*b*) since one of the axes is redundant, only directions [*uvtw*] having

$$u+v+t=0 \tag{3}$$

need to be recognized (Weber, 1922), and [*uvtw*] is parallel to (*hkil*) if and only if

$$hu+kv+it+lw=0\,. \tag{4}$$

The use of the redundant axes ${}_H\mathbf{a}_3 (=-{}_H\mathbf{a}_1-{}_H\mathbf{a}_2)$ and ${}_H\mathbf{a}_3^\dagger (=-{}_H\mathbf{a}_1^\dagger-{}_H\mathbf{a}_2^\dagger)$ is justified by the relatively simple crystallographic formulae that arise. Furthermore, Frank (1965) has shown how the hexagonal lattice and its reciprocal can be derived from four-dimensional orthogonal lattices whose obvious bases project to give ${}_H\mathbf{a}_i$, $\mathbf{c}$ and ${}_H\mathbf{a}_i^\dagger$, $\mathbf{c}^\dagger$ in three dimensions. Prior to Frank's paper, the basis of Miller–Bravais indexing seems never to have been examined with sufficient depth and rigour.

The aim of this paper is to consider the more general problem of introducing a redundant vector into the basis of any lattice, to show that a basis satisfying the analogue of equation (2) can always be found for the reciprocal lattice and indeed that this basis is not unique. The virtue of having such a relation is that the usefulness of the concept of the reciprocal lattice is

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carried through into this case. The problem is considered for n-dimensional space since such a generalization produces no significant increase in complexity; results for the hexagonal lattice are derived as an example. It is found that relation (4) is true under much less restrictive conditions than those prescribed above and, indeed, that it and its generalization are true provided only that the indices of a plane are defined as the reciprocals of its intercepts on the base vectors.

2. Preliminary comments about the hexagonal lattice

By virtue of equation (1), equation (2) can be rewritten as

$$\mathbf{h}=h({}_H\mathbf{a}_1^\dagger+\mathbf{d}^\dagger)+k({}_H\mathbf{a}_2^\dagger+\mathbf{d}^\dagger)+i({}_H\mathbf{a}_3^\dagger+\mathbf{d}^\dagger)+l\mathbf{c}^\dagger, \quad (5)$$

where $\mathbf{d}^\dagger$ is any vector, *i.e.* equation (2) is still valid when the reciprocal lattice is described by the basis ${}_H\mathbf{a}_i^\dagger+\mathbf{d}^\dagger$, $(i=1,2,3)$, $\mathbf{c}^\dagger$. This is contrary to the statement in Frank (1965) which implies that labelling the reciprocal lattice points by the indices of the planes to which they are normal determines a unique basis for the reciprocal lattice.

Similarly, equation (4) can be rewritten as

$$h(u+z)+k(v+z)+i(t+z)+lw=0\,, \quad (6)$$

where z is an arbitrary scalar, *i.e.* equation (4) is true for directions whose components do not satisfy equation (3). The special case of $z=-t$ reduces equation (6) to the form appropriate to indexing on the three-axis hexagonal (sometimes called monoclinic) system.

3. General case of a redundant axis

We will consider an n-dimensional space. To describe such space, n linearly-independent vectors are needed, but we will choose $(n+1)$ vectors $\mathbf{a}_i$ $(i=1,2,\ldots,n+1)$ so that one vector is redundant and precisely one linear relation exists between the $\mathbf{a}_i$. Let this relation be

$$\beta_i\mathbf{a}_i=0\,, \quad (7)$$

where the β_i are constants and a repeated suffix will be taken to imply summation over 1 to $n+1$. It is possible that some of the β_i are zero but this is ignored until the last part of this section where its effects are considered in detail.

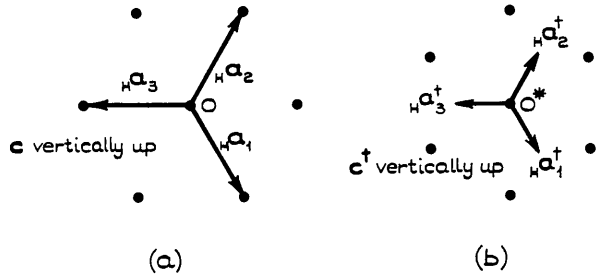

Fig. 1. Four-axis bases used for describing (*a*) the direct hexagonal lattice and (*b*) the corresponding reciprocal lattice.

If we now consider a hyperplane (hereafter abbreviated to plane) P in this space (Fig. 2) and suppose that

(A.1) P makes intercepts $1/h_i$ on the base vectors $\mathbf{a}_i$, *i.e.* passes through the points with position vectors $\mathbf{a}_1/h_1$, $\mathbf{a}_2/h_2$, *etc.*,

(A.2) $\mathbf{h}$ is a vector normal to P and of magnitude equal to the reciprocal of the distance, p, of P from the origin, and

(A.3) a typical vector in the space is of the form $\mathbf{u}=u_i\mathbf{a}_i$,

then the following questions are of interest.

Q.1. *What relation exists between the h_i?*

From Fig. 2, it is clear that

$$\mathbf{h}\,.\,(\mathbf{a}_1/h_1)=\mathbf{h}\,.\,(\mathbf{a}_2/h_2)=\ldots=p|\mathbf{h}|=1, \text{ by virtue of (A.2)}, \quad (8)$$

i.e.

$$\mathbf{h}\,.\,\mathbf{a}_i=h_i, \text{ for } i=1,2,\ldots,n+1\,. \quad (9)$$

Thus, by taking the scalar product of $\mathbf{h}$ with equation (7), we find

$$\mathbf{h}\,.\,\beta_i\mathbf{a}_i=\beta_i(\mathbf{h}\,.\,\mathbf{a}_i)=\beta_i h_i=0\,, \quad (10)$$

which is a linear relation between the h_i, and, since n of the h_i can be chosen arbitrarily, this is the only possible relation between the h_i.

Q.2. *What is the condition that $\mathbf{u}$ is parallel to the plane P?*

This condition is clearly

$$\mathbf{h}\,.\,\mathbf{u}=0\,, \quad (11)$$

and we can write

$$\begin{aligned}\mathbf{h}\,.\,\mathbf{u}&=\mathbf{h}\,.\,(u_i\mathbf{a}_i), \text{ by (A.3)},\\ &=(\mathbf{h}\,.\,\mathbf{a}_i)u_i,\\ &=h_iu_i, \text{ by (9)}.\end{aligned} \quad (12)$$

Thus,

$$h_iu_i=0 \quad (13)$$

is the required condition and this holds without any other restriction on the u_i; in particular, the analogue of equation (3) is not necessary for equation (13) [the analogue of equation (4)] to hold. In fact, equation (13) is true whenever the h_i are defined as reciprocal intercepts on the $\mathbf{a}_i$ and the u_i are defined conventionally.

Q.3. *Is it always possible to find a set of vectors $\mathbf{a}_i^\dagger$ such that, for any $\mathbf{h}$,*

$$\mathbf{h}=h_i\mathbf{a}_i^\dagger\,, \quad (14)$$

and, if so, what conditions must such vectors satisfy?

Clearly, one possible set is formed by choosing $\mathbf{a}_1^\dagger,\ldots,\mathbf{a}_n^\dagger$ to be a basis reciprocal to $\mathbf{a}_1,\ldots,\mathbf{a}_n$ and putting $\mathbf{a}_{n+1}^\dagger=0$, *i.e.* by simply ignoring $\mathbf{a}_{n+1}$. Further,

since the ordering of the $\mathbf{a}_i$ is arbitrary, other solutions can be found by a similar process based on any n of the $\mathbf{a}_i$. The question then becomes that of looking for the most general solution.

If equation (14) holds, equation (9) can be rewritten as

$$h_i\mathbf{a}_i^\dagger \cdot \mathbf{a}_j = h_j \tag{15}$$

i.e.

$$h_i(\mathbf{a}_i^\dagger \cdot \mathbf{a}_j - \delta_{ij}) = 0\,, \text{ for } j=1, \ldots, n+1\,. \tag{16}$$

Since each of the equations in the set (16) is a linear relation between the h_i, each must be equivalent to a linear multiple of equation (10), *i.e.*

$$\mathbf{a}_i^\dagger \cdot \mathbf{a}_j = \delta_{ij} + \beta_j^\dagger \beta_i\,, \tag{17}$$

where the $\beta_j^\dagger$ are a set of constants, as yet arbitrary, and (17) is a set of $(n+1)^2$ equations, each corresponding to a particular choice of i and j.

By taking all equations (17) with a particular i, multiplying each by its appropriate β_j and summing, we get

$$\begin{aligned}\mathbf{a}_i^\dagger \cdot \beta_j\mathbf{a}_j &= \beta_j\delta_{ij} + \beta_j\beta_j^\dagger\beta_i \\ &= \beta_i(1+\beta_j\beta_j^\dagger)\,.\end{aligned} \tag{18}$$

For each such equation (18), equation (7) implies that the left-hand side is zero and thus, either all β_i are zero (which is impossible) or

$$\beta_j^\dagger\beta_j + 1 = 0\,. \tag{19}$$

Thus, of the $n+1$ constants $\beta_j^\dagger$, n can be chosen arbitrarily and the last must then be chosen to satisfy equation (19).

Conversely, by taking all equations (17) with a particular j, multiplying each by its appropriate $\beta_i^\dagger$ and summing, we get

$$\begin{aligned}\beta_i^\dagger\mathbf{a}_i^\dagger \cdot \mathbf{a}_j &= \beta_i^\dagger(\delta_{ij} + \beta_i^\dagger\beta_i) \\ &= \beta_i^\dagger(1+\beta_i^\dagger\beta_i) = 0, \text{ by virtue of (19).}\end{aligned} \tag{20}$$

Thus, the vector sum $\beta_i^\dagger\mathbf{a}_i^\dagger$ is perpendicular to each of the $\mathbf{a}_j$ $(j=1, \ldots, n+1)$ and this can only be true if it is the null-vector, *i.e.*

$$\beta_i^\dagger\mathbf{a}_i^\dagger = 0\,. \tag{21}$$

Equation (21) is the analogue of equation (7) and shows that the $\beta_i^\dagger$ are related to the $\mathbf{a}_i^\dagger$ in the same way as the β_i are to the $\mathbf{a}_i$; this justifies the notation introduced at equation (17).

Equation (19) shows that we have n degrees of freedom in our choice of the $\mathbf{a}_i^\dagger$, a choice which can be exercised, for instance, by choosing the n scalars $\beta_1^\dagger, \ldots, \beta_n^\dagger$ say, or by arbitrarily fixing one of the vectors, say $\mathbf{a}_{n+1}^\dagger$. The special case of $\mathbf{a}_{n+1}^\dagger = 0$ implies that $\beta_1^\dagger = \ldots \beta_n^\dagger = 0$ and $\beta_{n+1}^\dagger\beta_{n+1} = -1$. Then equations (17) become

$$\mathbf{a}_i^\dagger \cdot \mathbf{a}_j = \delta_{ij}, \text{ for } i,j=1, \ldots, n\,, \tag{22}$$

i.e. the $\mathbf{a}_i^\dagger$ $(i=1, \ldots, n)$ are reciprocal to the $\mathbf{a}_j$ $(j=1, \ldots, n)$, *i.e.* we have the special solution given immediately after equation (14).

Q.4. *What is the geometrical significance of the $\beta_i^\dagger$ and of equations* (17)*?*

If we write, *without* using the summation convention,

$$\begin{aligned}\mathbf{A}_i^\dagger &= \mathbf{a}_i^\dagger/\beta_i\,, \\ \mathbf{A}_j &= \beta_j\mathbf{a}_j\,, \\ \theta_j &= \beta_j^\dagger\beta_j\,,\end{aligned} \tag{23}$$

then equations (17) become

$$\begin{aligned}\mathbf{A}_i^\dagger \cdot \mathbf{A}_j &= (\beta_j/\beta_i)\delta_{ij} + \theta_j \\ &= \delta_{ij} + \theta_j\,,\end{aligned} \tag{24}$$

and equation (19) becomes

$$\sum_{j=1}^{n+1} \theta_j = -1\,. \tag{25}$$

A geometric interpretation of all equations (24) with a given j can be obtained by drawing, in *reciprocal space*, planes P_j and Π_j normal to $\mathbf{A}_j$ and at distances $\theta_j/|\mathbf{A}_j|$ and $(1+\theta_j)/|\mathbf{A}_j|$ from the origin O^* (see Fig. 3). Then the equations (24) imply that all $\mathbf{A}_i^\dagger$ must extend from O^* to P_j except for $\mathbf{A}_j^\dagger$ which must extend to Π_j. If such constructions are carried through for all j, the intersection of Π_i and P_j (all $j \neq i$) will define the vector $\mathbf{A}_i^\dagger$, the relation (25) sufficing to ensure that these $n+1$ planes do meet in just one point. Thus, the end points of the $\mathbf{A}_i^\dagger$ define an $(n+1)$-hedron, in the reciprocal n-space, which is fixed in size and orientation (since each face is normal to an $\mathbf{A}_j^\dagger$ and the width normal to this face is just $|\mathbf{A}_j|^{-1}$) but can be located anywhere in reciprocal space by the appropriate choice of θ_j $(j=1, \ldots, n)$. This freedom of location allows the $\mathbf{A}_i^\dagger$, and hence the $\mathbf{a}_i^\dagger$, to be chosen to fit, for instance, some desirable symmetry condition such as is prescribed below.

Q.5. *Under what conditions are symmetricallyrelated directions indexed equivalently?*

The original aim of introducing a redundant axis was to obtain a symmetrical notation, *i.e.* the aim was that symmetricallyrelated planes and directions would have

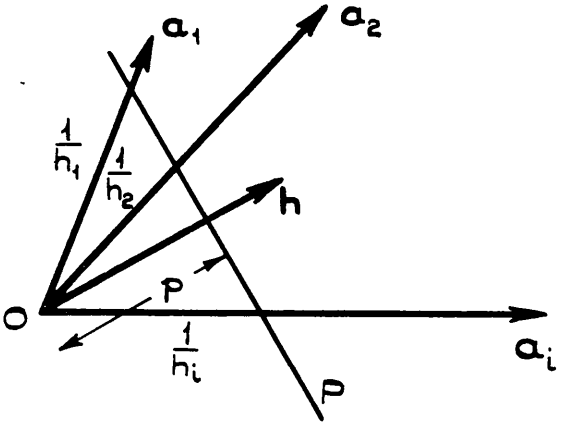

Fig. 2. Hyperplane P and its intersections on base axes.

symmetricallyrelated indices. Since the indices of planes are defined by the reciprocal intercepts on the $\mathbf{a}_i$, this aim for planes will be achieved by choosing a symmetrical set of $\mathbf{a}_i$, *i.e.* by ensuring that the 'axial cross', constructed from the $\mathbf{a}_i$ and their negatives, shows the required point symmetry. However, the situation for directions is not so obvious.

Any point in space can be described by $n+1$ coordinates u_i in a variety of ways, and to achieve symmetrical descriptions this redundancy must first be removed by imposing some condition on the u_i. Clearly, it is desirable that the condition should allow the coordinates to be added as vector components, *i.e.* that if

$$\mathbf{u}+\mathbf{u}'=\mathbf{u}'' \tag{26}$$

then

$$u_i+u_i'=u_i'', \quad \text{for all } i. \tag{27}$$

A consideration of the properties of linear functions shows that this result is true if and only if the relation between the u_i is linear and homogeneous, *i.e.* it must be of the form

$$\alpha_i u_i=0\,, \tag{28}$$

where the α_i are constants as yet unspecified.

A simple method of attaining the desired equivalence is to demand a relation between directions in real space and planes in reciprocal space similar to that already exisiting between real planes and reciprocal directions and then, by a suitable choice of $\mathbf{a}_i^\dagger$, to ensure that equivalent planes in reciprocal space are equivalently indexed. This implies that the $\mathbf{a}_i^\dagger$ must be chosen to reflect the symmetry required, *i.e.* must have the same symmetry as the $\mathbf{a}_i$. The duality condition implies that a plane in reciprocal space making intercepts of u_i^{-1} on the $\mathbf{a}_i^\dagger$ has, as normal, the vector*

$$\mathbf{u}=u_i\mathbf{a}_i\,. \tag{29}$$

Hence an argument analogous to that leading from equation (7) to equation (10) shows that equation (21) implies that equation (28), the condition on the u_i, is in fact

$${}_s\beta_i^\dagger u_i=0\,, \tag{30}$$

where the ${}_s\beta_i^\dagger$ are the particular $\beta_i^\dagger$ that correspond to the symmetric choice of $\mathbf{a}_i^\dagger$.

Since equation (30) alone suffices to ensure the equivalent indexing of directions, the duality condition and the consequent restriction on the $\mathbf{a}_i^\dagger$, used in deriving the ${}_s\beta_i^\dagger$, are not essential. However, since nothing is gained by dropping these latter conditions, in practice it is sensible to retain them. It should be stressed here that the truth of equation (13) does not imply duality, contrary to the statement in Frank (1965).

Q.6. *How do lattice properties enter the problem?*

The above analysis has taken no account of lattice properties and indeed holds true for general points and planes in n-space. When, however, we are concerned with an n-dimensional lattice, L say, the $\mathbf{a}_i$ should be chosen so that all lattice vectors are expressible as rational multiples of the $\mathbf{a}_i$ and this implies that the β_i are rational and may, if desired, be chosen as a set of integers without a common factor.

If P is taken as the plane of given orientation that passes through lattice points and passes as close as

* Complete consistency of notation could have been achieved by writing $\mathbf{u}$ and u_i as $\mathbf{h}^\dagger$ and $h_i{}^\dagger$ but this would have been confusing as it conflicts with conventional crystallographic practice.

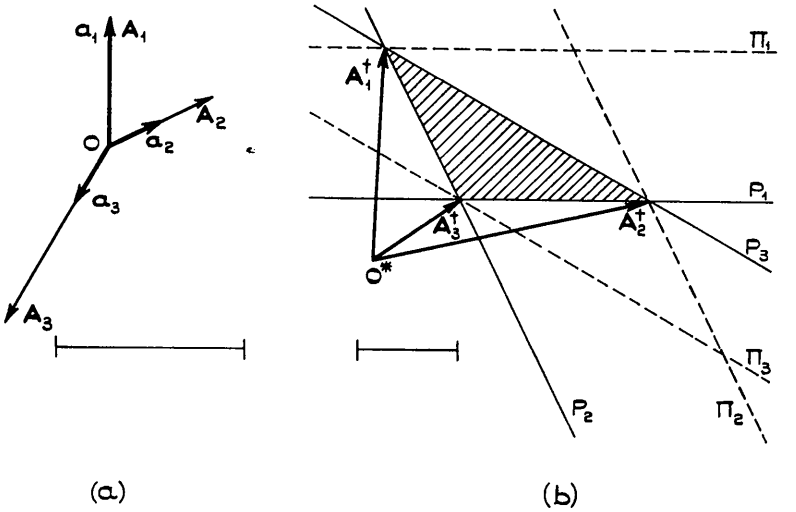

Fig. 3. Geometrical construction for finding a set of $\mathbf{a}_i{}^\dagger$ satisfying $\mathbf{h}=h_i\mathbf{a}_i{}^\dagger$ from a given set of $\mathbf{a}_i$. The relative scales of (*a*) direct and (*b*) reciprocal space are shown. To obtain $\mathbf{a}_i{}^\dagger$ from the Figure, each $\mathbf{A}_i{}^\dagger$ must be multiplied by the corresponding β_i. Other sets of $\mathbf{A}_i{}^\dagger$ (and hence $\mathbf{a}_i{}^\dagger$) can be found by translating the shaded triangle in (*b*). The diagram has been drawn for the particular relation $\mathbf{a}_1+2\mathbf{a}_2+3\mathbf{a}_3=0$ and for $\theta_1=0{\cdot}4$, $\theta_2=0{\cdot}6$, $\theta_3=-2{\cdot}0$.

possible to O without including it, then the h_i can be written in the form

$$h_i = qh'_i \,, \tag{31}$$

where q is rational and the h'_i are a set of integers without a common factor that are the n-dimensional analogues of Miller–Bravais indices for the plane.*

If we now consider the lattice reciprocal to L, say L^*, then *any* basis $\mathbf{a}_i^\dagger$ that satisfies equations (17) is a satisfactory basis for L^* in that equation (14) will be satisfied and all reciprocal lattice vectors will be rational multiples of the base vectors. If the β_i have been chosen as integers without a common factor then equation (19) ensures that it will always be possible to choose $\beta_i^\dagger$ with the same properties. However, such a choice may conflict with symmetry requirements such as are discussed in Q.5; if so, then we may have to be satisfied with restricting the $\beta_i^\dagger$ to rational values.

Q.7. *What complications arise if some of the β_i are zero?*

If some of the β_i are zero, modification is needed to parts of the previous argument. Suppose that all such β_i are denoted by β_r, $r=1, \ldots, l$. Then, the difficulties could be overcome by temporarily removing the corresponding $\mathbf{a}_r$ from consideration, working in $(n-l)$-dimensional space, and finally recovering the $\mathbf{a}_r$, but it seems simpler to consider each modification individually.

(i) In the argument immediately following equation (14), the set $\mathbf{a}_1, \ldots, \mathbf{a}_n$ must include all $\mathbf{a}_r$.

(ii) When choosing $\beta_i^\dagger$ to satisfy equation (19), the n arbitrarily chosen constants must include all $\beta_r^\dagger$.

(iii) In equation (23), any $\mathbf{A}_r$ would be infinite. Detailed consideration shows that for just one zero β_r, the $(n+1)$-hedron becomes a prism with generators normal to all $\mathbf{a}_i$ $(i \neq r)$, $\mathbf{a}_r^\dagger$ is parallel to these generators and of magnitude $|\mathbf{a}_r|^{-1}$, and the other $\mathbf{A}_i$ end at the vertices of the n-gon formed by the intersection of the prism with a plane perpendicular to $\mathbf{a}_r$. The n degrees of freedom available in choosing the $\mathbf{a}_i^\dagger$ then comprise the $n-1$ degrees available for locating the prism and one for locating the plane. A similar argument can be devised for more than one zero β_i, but it is difficult to express geometrically.

(iv) In determining the limits of q for use in equation (31), the only unit cells considered are those which include all $\mathbf{a}_r$.

4. Application to the hexagonal lattice

Since the point symmetry of the hexagonal lattice is 6/*mmm*, the 'axial cross' of the $\mathbf{a}_i$ should by Q.5 show such symmetry and the only possible systems are:

$$\begin{aligned} &\mathbf{a}_i = C\,{}_H\mathbf{a}_i \,, \qquad i=1,2,3 \,, \\ &\mathbf{a}_4 = D\mathbf{c} \,, \end{aligned} \tag{32}$$

or

$$\begin{aligned} &\mathbf{a}_1 = C'({}_H\mathbf{a}_2 - {}_H\mathbf{a}_3), \; etc. \\ &\mathbf{a}_4 = D'\mathbf{c} \,, \end{aligned} \tag{33}$$

where ${}_H\mathbf{a}_i$, $\mathbf{c}$ are as in Fig. 1(*a*) and C, D, C', D' are arbitrary constants.

The convenient, and conventional, choice is of course to adopt equations (32) with $C=D=1$. Then, in the notation of § 3,

$$\mathbf{a}_1+\mathbf{a}_2+\mathbf{a}_3 = {}_H\mathbf{a}_1+{}_H\mathbf{a}_2+{}_H\mathbf{a}_3 = 0 \tag{34}$$

i.e.

$$\beta_1=\beta_2=\beta_3=1 \text{ and } \beta_4=0 \,. \tag{35}$$

Using (*hkil*) as indices of a plane, equation (10) gives the well-known result

$$h+k+i+(0.l)=0 \tag{1}$$

and equation (4) follows immediately from equation (13) with $u_i=[uvtw]$, and no special conditions on u, v, t, w.

Now, application of equations (17) shows that equation (5), the special case of equation (14), will be true for *any* basis satisfying

$$\begin{aligned} &\mathbf{a}_i^\dagger = {}_H\mathbf{a}_i^\dagger + \mathbf{d}^\dagger, \qquad i=1,2,3 \,, \\ &\mathbf{a}_4^\dagger = \mathbf{c}^\dagger, \end{aligned} \tag{36}$$

where ${}_H\mathbf{a}_i^\dagger$ and $\mathbf{c}^\dagger$ are given in Fig. 1(*b*), and $\mathbf{d}^\dagger$ is an arbitrary vector in reciprocal space, not necessarily coplanar with ${}_H\mathbf{a}_i^\dagger$. The analysis in Q.7(iii) shows that $\mathbf{a}_4^\dagger$ is uniquely determined.

In order to find the condition leading to symmetrical representation of directions, we make use of an axial cross of the $\mathbf{a}_i^\dagger$ which displays the symmetry of the reciprocal lattice, namely 6/*mmm*. This is achieved by putting $\mathbf{d}^\dagger=0$ so that we have

$$\mathbf{a}_1^\dagger+\mathbf{a}_2^\dagger+\mathbf{a}_3^\dagger = {}_H\mathbf{a}_1^\dagger+{}_H\mathbf{a}_2^\dagger+{}_H\mathbf{a}_3^\dagger = 0 \,. \tag{37}$$

Thus, from equations (19) and (21),

$$\beta_1^\dagger=\beta_2^\dagger=\beta_3^\dagger=-\tfrac{1}{3} \text{ and } \beta_4^\dagger=0 \,. \tag{38}$$

From equation (30), we now can deduce that to achieve the symmetrical representation of directions we need

$$u+v+t=0 \,. \tag{3}$$

Finally, if we desire duality between the treatment of the direct and reciprocal lattices we choose as basis for the reciprocal lattice the symmetric basis of ${}_H\mathbf{a}_i^\dagger$, $\mathbf{c}^\dagger$, which is derived from equations (36) by putting $\mathbf{d}^\dagger=0$. Fig. 1(*b*) shows that the relation between the axial cross of ${}_H\mathbf{a}_i^\dagger$ and the shortest lattice vectors in the reciprocal lattice is analogous to equations (33) with $C'=\frac{1}{3}$ and $D'=1$, rather than to equations (32).

* In order to determine possible values of q, and q may vary from plane to plane, we first calculate the ratio of the volume of a primitive unit cell in the lattice to the volume of the unit cell defined by each set of n of the $\mathbf{a}_i$. Let the greatest and least ratios be $Q_{\max}$ and $Q_{\min}$. Then if $Q_{\max} \geq 1$, $Q_{\max}/q$ must be integral and if $Q_{\min} \leq 1$, $q/Q_{\min}$ must be integral; if $Q_{\max} < 1$, then $q \leq 1$ and if $Q_{\min} > 1$, $q \geq 1$.

5. Conclusion

The detailed argument above was not intended to suggest alternative methods of indexing the hexagonal system but rather to show why and when each particular choice of axes and indices is needed. The argument has incidentally shown that there is no alternative method having all the advantages of the Miller–Bravais system. Our general conclusions, of which (*c*) and (*d*) run counter to common assumptions, can be summarized as follows:

(*a*) a symmetric basis for the direct lattice is necessary for the equivalent indexing of symmetrically-related planes;

(*b*) the use of a redundant axis implies that a linear relation exists between the indices of a plane, this relation being equation (10) in the general case or, for the hexagonal lattice,

$$h+k+i=0; \tag{1}$$

(*c*) the equation

$$\mathbf{h} \,.\, \mathbf{u}=h_i u_i \tag{12}$$

[and hence equation (4) for the hexagonal lattice] holds irrespective of the bases chosen and its validity implies nothing about 'best' choices nor about duality nor about equivalent indexing of planes and directions;

(*d*) it is always possible to find a basis $\mathbf{a}_i^\dagger$ ($i=1, \ldots, n+1$) for the reciprocal lattice such that

$$\mathbf{h}=h_i \mathbf{a}_i^\dagger \tag{14}$$

but the validity of this equation is not sufficient to define a unique basis;

(*e*) the equivalent indexing of symmetrically related directions implies that the indices of a direction must satisfy a linear relationship such as equation (30), *e.g.* for the hexagonal lattice

$$u+v+t=0; \tag{3}$$

(*f*) duality between planes and directions in direct and reciprocal space can be made the final determinant of the choice of a reciprocal basis after symmetry conditions have been satisfied.

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The Variation with Wavelength of the Atomic Scattering Factor for Iron

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The atomic scattering factor for iron has been measured on five low-order reflexions from pure iron at eighteen wavelengths in the range 0·63 to 2·53 Å; measurements have also been made on nickel for Cu $K\alpha$ radiation to give additional checks with results of other workers. The variation of f for iron follows the Hönl theory for K-electrons quite closely, except for the 110 reflexion at wavelengths just short of the absorption edge. The dispersion corrections were independent of angle. The limiting values of f at high frequencies indicated by the results agree well with other theoretical and experimental values, except for the 110 reflexion.

1. Introduction

Measurements of the atomic scattering factor f as a function of wavelength determine the dispersion correction δf if a value of f_0, the limiting value for very high frequencies, can be assumed. The relation between f, f_0 and δf is

$$\delta f=|f|-f_0 \simeq \Delta f'+\frac{(\Delta f'')^2}{2(f_0+\Delta f')}$$

$\Delta f'$ and $\Delta f''$ are the in-phase and out-of-phase parts of the dispersion term: in the present work, the wavelength variation of $|f|$ has been measured and no separate determination of $\Delta f'$ and $\Delta f''$ has been attempted.

The theory of anomalous dispersion effects shows how $\Delta f'$ and $\Delta f''$ can be calculated in terms of the oscillator strengths of the electron shells (see, for example, James, 1962). These in turn can be computed from atomic wave functions (Hönl, 1933*a*,*b*) or from