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3.1.3. Reduced bases

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3.1.3.1. Introduction

Unit cells are usually chosen according to the conventions mentioned in Section 3.1.1, so one might think that there is no need for another standard choice. This is not true, however; conventions based on symmetry do not always permit unambiguous choice of the unit cell, and unconventional descriptions of a lattice do occur. They are often chosen for good reasons or they may arise from experimental limitations such as may occur, for example, in high-pressure work. So there is a need for normalized descriptions of crystal lattices.

Accordingly, the *reduced basis*[1] (Eisenstein, 1851; Niggli, 1928), which is a primitive basis unique (apart from orientation) for any given lattice, is at present widely used as a means of classifying and identifying crystalline materials. A comprehensive survey of the principles, the techniques and the scope of such applications is given by Mighell (1976). The present contribution merely aims at an exposition of the basic concepts and a brief account of some applications.

The main criterion for the reduced basis is a metric one: choice of the shortest three non-coplanar lattice vectors as basis vectors. Therefore, the resulting bases are, in general, widely different from any symmetry-controlled basis, *cf.* Section 3.1.1.

3.1.3.2. Definition

A primitive basis **a**, **b**, **c** is called a 'reduced basis' if it is right-handed and if the components of the metric tensor ***G*** (*cf.* Section 3.1.1)

$$\begin{matrix} \mathbf{a}\cdot\mathbf{a} & \mathbf{b}\cdot\mathbf{b} & \mathbf{c}\cdot\mathbf{c} \\ \mathbf{b}\cdot\mathbf{c} & \mathbf{c}\cdot\mathbf{a} & \mathbf{a}\cdot\mathbf{b} \end{matrix} \qquad (3.1.3.1)$$

satisfy the conditions shown below. The matrix (3.1.3.1) for the reduced basis is called the *reduced form*.

Because of lattice symmetry there can be two or more possible orientations of the reduced basis in a given lattice but, apart from orientation, the reduced basis is unique.

Any basis, reduced or not, determines a unit cell – that is, the parallelepiped of which the basis vectors are edges. In order to test whether a given basis is the reduced one, it is convenient first to find the 'type' of the corresponding unit cell. The type of a cell depends on the sign of

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

If $T > 0$, the cell is of type I, if $T \le 0$ it is of type II. 'Type' is a property of the cell since T keeps its value when **a**, **b** or **c** is inverted. Geometrically speaking, such an inversion corresponds to moving the origin of the basis towards another corner of the cell. Corners with all three angles acute occur for cells of type I (one opposite pair, the remaining six corners having one acute and two obtuse angles). The other alternative, specified by main condition (ii) of Section 3.1.3.3, *viz* all three angles non-acute, occurs for cells of type II (one or more opposite pairs, the remaining corners having either one or two acute angles).

The conditions can all be stated analytically in terms of the components (3.1.3.1), as follows:

(*a*) Type-I cell

Main conditions:

$$\mathbf{a}\cdot\mathbf{a} \le \mathbf{b}\cdot\mathbf{b} \le \mathbf{c}\cdot\mathbf{c};\quad |\mathbf{b}\cdot\mathbf{c}| \le \tfrac{1}{2}\mathbf{b}\cdot\mathbf{b};\quad |\mathbf{a}\cdot\mathbf{c}| \le \tfrac{1}{2}\mathbf{a}\cdot\mathbf{a};\quad |\mathbf{a}\cdot\mathbf{b}| \le \tfrac{1}{2}\mathbf{a}\cdot\mathbf{a} \qquad (3.1.3.2a)$$

$$\mathbf{b}\cdot\mathbf{c} > 0;\quad \mathbf{a}\cdot\mathbf{c} > 0;\quad \mathbf{a}\cdot\mathbf{b} > 0. \qquad (3.1.3.2b)$$

Special conditions:

$$\text{if}\quad \mathbf{a}\cdot\mathbf{a} = \mathbf{b}\cdot\mathbf{b}\quad \text{then}\quad \mathbf{b}\cdot\mathbf{c} \le \mathbf{a}\cdot\mathbf{c} \qquad (3.1.3.3a)$$

$$\text{if}\quad \mathbf{b}\cdot\mathbf{b} = \mathbf{c}\cdot\mathbf{c}\quad \text{then}\quad \mathbf{a}\cdot\mathbf{c} \le \mathbf{a}\cdot\mathbf{b} \qquad (3.1.3.3b)$$

$$\text{if}\quad \mathbf{b}\cdot\mathbf{c} = \tfrac{1}{2}\mathbf{b}\cdot\mathbf{b}\quad \text{then}\quad \mathbf{a}\cdot\mathbf{b} \le 2\mathbf{a}\cdot\mathbf{c} \qquad (3.1.3.3c)$$

$$\text{if}\quad \mathbf{a}\cdot\mathbf{c} = \tfrac{1}{2}\mathbf{a}\cdot\mathbf{a}\quad \text{then}\quad \mathbf{a}\cdot\mathbf{b} \le 2\mathbf{b}\cdot\mathbf{c} \qquad (3.1.3.3d)$$

$$\text{if}\quad \mathbf{a}\cdot\mathbf{b} = \tfrac{1}{2}\mathbf{a}\cdot\mathbf{a}\quad \text{then}\quad \mathbf{a}\cdot\mathbf{c} \le 2\mathbf{b}\cdot\mathbf{c}. \qquad (3.1.3.3e)$$

(*b*) Type-II cell

Main conditions:

$$\text{as (3.1.3.2}a) \qquad (3.1.3.4a)$$

$$(|\mathbf{b}\cdot\mathbf{c}| + |\mathbf{a}\cdot\mathbf{c}| + |\mathbf{a}\cdot\mathbf{b}|) \le \tfrac{1}{2}(\mathbf{a}\cdot\mathbf{a} + \mathbf{b}\cdot\mathbf{b}) \qquad (3.1.3.4b)$$

$$\mathbf{b}\cdot\mathbf{c} \le 0;\quad \mathbf{a}\cdot\mathbf{c} \le 0;\quad \mathbf{a}\cdot\mathbf{b} \le 0. \qquad (3.1.3.4c)$$

Special conditions:

$$\text{if}\quad \mathbf{a}\cdot\mathbf{a} = \mathbf{b}\cdot\mathbf{b}\quad \text{then}\quad |\mathbf{b}\cdot\mathbf{c}| \le |\mathbf{a}\cdot\mathbf{c}| \qquad (3.1.3.5a)$$

$$\text{if}\quad \mathbf{b}\cdot\mathbf{b} = \mathbf{c}\cdot\mathbf{c}\quad \text{then}\quad |\mathbf{a}\cdot\mathbf{c}| \le |\mathbf{a}\cdot\mathbf{b}| \qquad (3.1.3.5b)$$

$$\text{if}\quad |\mathbf{b}\cdot\mathbf{c}| = \tfrac{1}{2}\mathbf{b}\cdot\mathbf{b}\quad \text{then}\quad \mathbf{a}\cdot\mathbf{b} = 0 \qquad (3.1.3.5c)$$

$$\text{if}\quad |\mathbf{a}\cdot\mathbf{c}| = \tfrac{1}{2}\mathbf{a}\cdot\mathbf{a}\quad \text{then}\quad \mathbf{a}\cdot\mathbf{b} = 0 \qquad (3.1.3.5d)$$

$$\text{if}\quad |\mathbf{a}\cdot\mathbf{b}| = \tfrac{1}{2}\mathbf{a}\cdot\mathbf{a}\quad \text{then}\quad \mathbf{a}\cdot\mathbf{c} = 0 \qquad (3.1.3.5e)$$

$$\text{if}\quad (|\mathbf{b}\cdot\mathbf{c}| + |\mathbf{a}\cdot\mathbf{c}| + |\mathbf{a}\cdot\mathbf{b}|) = \tfrac{1}{2}(\mathbf{a}\cdot\mathbf{a} + \mathbf{b}\cdot\mathbf{b})\quad \text{then}\quad \mathbf{a}\cdot\mathbf{a} \le 2|\mathbf{a}\cdot\mathbf{c}| + |\mathbf{a}\cdot\mathbf{b}|. \qquad (3.1.3.5f)$$

The geometrical interpretation in the following sections is given in order to make the above conditions more explicit rather than to replace them, since the analytical form is obviously the most suitable one for actual verification.

3.1.3.3. Main conditions

The main conditions[2] express the following two requirements:

(i) Of all lattice vectors, none is shorter than **a**; of those not directed along **a**, none is shorter than **b**; of those not lying in the **ab** plane, none is shorter than **c**. This requirement is expressed analytically by (3.1.3.2*a*), and for type-II cells by (3.1.3.4*b*), which for type-I cells is redundant.

(ii) The three angles between basis vectors are either all acute or all non-acute, conditions (3.1.3.2*b*) and (3.1.3.4*c*). As shown in Section 3.1.3.2 for a given unit cell, the origin corner can always be chosen so as to satisfy either the first alternative of this condition (if the cell is of type I) or the second (if the cell is of type II).

[1] Very often, the term 'reduced cell' is used to indicate this normalized lattice description. To avoid confusion, we shall use 'reduced basis', since it is actually a basis and some of the criteria are related precisely to the difference between unit cells and vector bases.

[2] In a book on reduced cells and on retrieval of symmetry information from lattice parameters, Gruber (1978) reformulated the main condition (i) as a minimum condition on the sum $s = a + b + c$. He also examined the surface areas of primitive unit cells in a given lattice, which are easily shown to be proportional to the corresponding sums $s^* = a^* + b^* + c^*$ for the reciprocal bases. He finds that if there are two or more non-congruent cells with minimum s ('Buerger cells'), these cells always have different values of s^*. Gruber (1989) proposes a new criterion to replace the conditions (3.1.3.2*a*)–(3.1.3.5*f*), *viz* that, among the cells with the minimum s value, the one with the smallest value of s^* be chosen (which need not be the absolute minimum of s^* since that may occur for cells that are not Buerger cells). The analytic form of this criterion is identical to (3.1.3.2*a*)–(3.1.3.5*e*); only (3.1.3.5*f*) is altered. For further details, see Section 3.1.4.

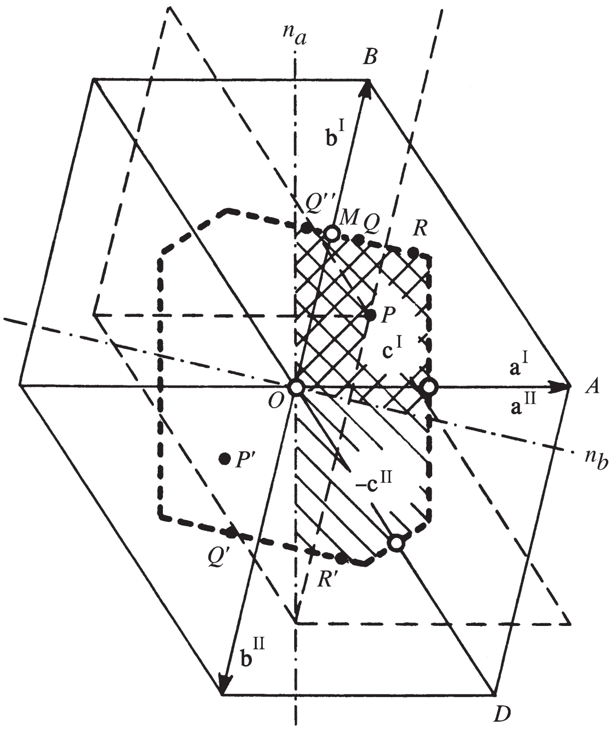

Figure 3.1.3.1
The net of lattice points in the plane of the reduced basis vectors **a** and **b**; *OBAD* is a primitive mesh. The actual choice of **a** and **b** depends on the position of the point *P*, which is the projection of the point P_0 in the next layer (supposed to lie above the paper, thin dashed lines) closest to *O*. Hence, *P* is confined to the Voronoi domain (dashed hexagon) around *O*. For a given interlayer distance, *P* defines the complete lattice. In that sense, *P* and *P'* represent identical lattices; so do *Q*, *Q'* and *Q''*, and also *R* and *R'*. When *P* lies in a region marked $-c^{\rm II}$ (hatched), the reduced type-II basis is formed by $\mathbf{a}^{\rm II}$, $\mathbf{b}^{\rm II}$ and $\mathbf{c} = -\overrightarrow{OP}_0$. Regions marked $c^{\rm I}$ (cross-hatched) have the reduced type-I basis $\mathbf{a}^{\rm I}$, $\mathbf{b}^{\rm I}$ and $\mathbf{c} = +\overrightarrow{OP}_0$. Small circles in *O*, *M etc.* indicate twofold rotation points lying on the region borders (see text).

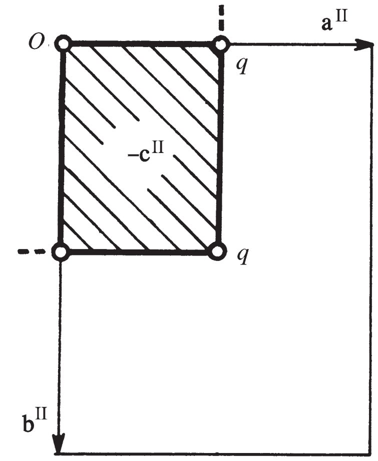

Figure 3.1.3.2
The effect of the special conditions. Border lines of type-I and type-II regions are drawn as heavy lines if included. The type-I and type-II regions are marked as in Fig. 3.1.3.1. A heavy border line of a region stops short of an end point if the latter is not included in the region to which the border belongs. **a**, **b** net primitive orthogonal; special conditions (3.1.3.5*c*), (3.1.3.5*d*).

Condition (i) is by far the most essential one. It uniquely defines the lengths *a*, *b* and *c*, and limits the angles to the range $60 \le \alpha, \beta, \gamma \le 120^\circ$. However, there are often different unit cells satisfying (i), *cf.* Gruber (1973). In order to find the reduced basis, starting from an arbitrary one given by its matrix (3.1.3.1), one can: (*a*) find some basis satisfying (i) and (ii) and if necessary modify it so as to fulfil the special conditions as well; (*b*) find all bases satisfying (i) and (ii) and test them one by one with regard to the special conditions until the reduced form is found. Method (*a*) relies mainly on an algorithm by Buerger (1957, 1960), *cf.* also Mighell (1976). Method (*b*) stems from a theorem and an algorithm, both derived by Delaunay (1933); the theorem states that the desired basis vectors **a**, **b** and **c** are among seven (or fewer) vectors – the distance vectors between parallel faces of the Voronoi domain – which follow directly from the algorithm. The method has been established and an example is given by Delaunay *et al.* (1973), *cf.* Section 3.1.2.3 where this method is described.

3.1.3.4. Special conditions

For a given lattice, the main condition (i) defines not only the lengths *a*, *b*, *c* of the reduced basis vectors but also the plane containing **a** and **b**, in the sense that departures from special conditions can be repaired by transformations which do not change this plane. An exception can occur when $b = c$; then such transformations must be supplemented by interchange(s) of **b** and **c** whenever either (3.1.3.3*b*) or (3.1.3.5*b*) is not fulfilled. All the other conditions can be conveniently illustrated by projections of part of the lattice onto the **ab** plane as shown in Figs. 3.1.3.1 to 3.1.3.5. Let us represent the vector lattice by a point lattice. In Fig. 3.1.3.1, the net in the **ab** plane (of which *OBAD* is a primitive mesh; $OA = a$, $OB = b$) is shown as well as the projection (normal to that plane) of the adjoining layer which is assumed to lie above the paper. In general, just one lattice node P_0 of that layer, projected in Fig. 3.1.3.1 as *P*, will be closer to the origin than all others. Then the vector $\overrightarrow{OP}_0$ is $\pm\mathbf{c}$ according to condition (i). It should be stressed that, though the **ab** plane is most often (see above) correctly established by (i), the vectors **a**, **b** and **c** still have to be chosen so as to comply with (ii), with the special conditions, and with right-handedness. The result will depend on the position of *P* with respect to the net. This dependence will now be investigated.

The inner hexagon shown, which is the two-dimensional Voronoi domain around *O*, limits the possible projected positions *P* of P_0. Its short edges, normal to *OD*, result from (3.1.3.4*b*); the other edges from (3.1.3.2*a*). If the spacing *d* between **ab** net planes is smaller than *b*, the region allowed for *P* is moreover limited inwardly by the circle around *O* with radius $(b^2 - d^2)^{1/2}$, corresponding to the projection of points P_0 for which $OP_0 = c = b$. The case $c = b$ has been dealt with, so in order to simplify the drawings we shall assume $d > b$. Then, for a given value of *d*, each point within the above-mentioned hexagonal domain, regarded as the projection of a lattice node P_0 in the next layer, completely defines a lattice based on $\overrightarrow{OA}$, $\overrightarrow{OB}$ and $\overrightarrow{OP}_0$. Diametrically opposite points like *P* and *P'* represent the same lattice in two orientations differing by a rotation of 180° in the plane of the figure. Therefore, the systematics of reduced bases can be shown completely in just half the domain. As a halving line, the n_a normal to *OA* is chosen. This is an important boundary in view of condition (ii), since it separates points *P* for which the angle between OP_0 and *OA* is acute from those for which it is obtuse.

Similarly, n_b, normal to *OB*, separates the sharp and obtuse values of the angles P_0OB. It follows that if *P* lies in the obtuse sector (cross-hatched area) between n_a and n_b, the reduced cell is

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