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9.2. Reduced bases

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9.2.1. Introduction

Unit cells are usually chosen according to the conventions mentioned in Chapter 9.1 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** (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.* Chapter 9.1.

9.2.2. Definition

A primitive basis $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$ is called a 'reduced basis' if it is right-handed and if the components of the metric tensor $\mathbf{G}$ (*cf.* Chapter 9.1)

$$\begin{matrix} \mathbf{a}\cdot\mathbf{a} & \mathbf{b}\cdot\mathbf{b} & \mathbf{c}\cdot\mathbf{c} \\ \mathbf{b}\cdot\mathbf{c} & \mathbf{c}\cdot\mathbf{a} & \mathbf{a}\cdot\mathbf{b} \end{matrix} \qquad (9.2.2.1)$$

satisfy the conditions shown below. The matrix (9.2.2.1) 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 $\mathbf{a}$, $\mathbf{b}$ or $\mathbf{c}$ 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 9.2.3, *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 (9.2.2.1), as follows:

* 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.

(*a*) Type-I cell

Main conditions:

$$\mathbf{a}\cdot\mathbf{a} \le \mathbf{b}\cdot\mathbf{b} \le \mathbf{c}\cdot\mathbf{c};\ |\mathbf{b}\cdot\mathbf{c}| \le \tfrac{1}{2}\mathbf{b}\cdot\mathbf{b};\ |\mathbf{a}\cdot\mathbf{c}| \le \tfrac{1}{2}\mathbf{a}\cdot\mathbf{a};\ |\mathbf{a}\cdot\mathbf{b}| \le \tfrac{1}{2}\mathbf{a}\cdot\mathbf{a} \qquad (9.2.2.2a)$$

$$\mathbf{b}\cdot\mathbf{c} > 0; \qquad \mathbf{a}\cdot\mathbf{c} > 0; \qquad \mathbf{a}\cdot\mathbf{b} > 0. \qquad (9.2.2.2b)$$

Special conditions:

$$\text{if } \mathbf{a}\cdot\mathbf{a} = \mathbf{b}\cdot\mathbf{b} \text{ then } \mathbf{b}\cdot\mathbf{c} \le \mathbf{a}\cdot\mathbf{c} \qquad (9.2.2.3a)$$

$$\text{if } \mathbf{b}\cdot\mathbf{b} = \mathbf{c}\cdot\mathbf{c} \text{ then } \mathbf{a}\cdot\mathbf{c} \le \mathbf{a}\cdot\mathbf{b} \qquad (9.2.2.3b)$$

$$\text{if } \mathbf{b}\cdot\mathbf{c} = \tfrac{1}{2}\mathbf{b}\cdot\mathbf{b} \text{ then } \mathbf{a}\cdot\mathbf{b} \le 2\mathbf{a}\cdot\mathbf{c} \qquad (9.2.2.3c)$$

$$\text{if } \mathbf{a}\cdot\mathbf{c} = \tfrac{1}{2}\mathbf{a}\cdot\mathbf{a} \text{ then } \mathbf{a}\cdot\mathbf{b} \le 2\mathbf{b}\cdot\mathbf{c} \qquad (9.2.2.3d)$$

$$\text{if } \mathbf{a}\cdot\mathbf{b} = \tfrac{1}{2}\mathbf{a}\cdot\mathbf{a} \text{ then } \mathbf{a}\cdot\mathbf{c} \le 2\mathbf{b}\cdot\mathbf{c}. \qquad (9.2.2.3e)$$

(*b*) Type-II cell

Main conditions:

$$\text{as } (9.2.2.2a) \qquad (9.2.2.4a)$$

$$(|\mathbf{b}\cdot\mathbf{c}| + |\mathbf{a}\cdot\mathbf{c}| + |\mathbf{a}\cdot\mathbf{b}|) \le \tfrac{1}{2}(\mathbf{a}\cdot\mathbf{a} + \mathbf{b}\cdot\mathbf{b}) \qquad (9.2.2.4b)$$

$$\mathbf{b}\cdot\mathbf{c} \le 0; \qquad \mathbf{a}\cdot\mathbf{c} \le 0; \qquad \mathbf{a}\cdot\mathbf{b} \le 0. \qquad (9.2.2.4c)$$

Special conditions:

$$\text{if } \mathbf{a}\cdot\mathbf{a} = \mathbf{b}\cdot\mathbf{b} \text{ then } |\mathbf{b}\cdot\mathbf{c}| \le |\mathbf{a}\cdot\mathbf{c}| \qquad (9.2.2.5a)$$

$$\text{if } \mathbf{b}\cdot\mathbf{b} = \mathbf{c}\cdot\mathbf{c} \text{ then } |\mathbf{a}\cdot\mathbf{c}| \le |\mathbf{a}\cdot\mathbf{b}| \qquad (9.2.2.5b)$$

$$\text{if } |\mathbf{b}\cdot\mathbf{c}| = \tfrac{1}{2}\mathbf{b}\cdot\mathbf{b} \text{ then } \mathbf{a}\cdot\mathbf{b} = 0 \qquad (9.2.2.5c)$$

$$\text{if } |\mathbf{a}\cdot\mathbf{c}| = \tfrac{1}{2}\mathbf{a}\cdot\mathbf{a} \text{ then } \mathbf{a}\cdot\mathbf{b} = 0 \qquad (9.2.2.5d)$$

$$\text{if } |\mathbf{a}\cdot\mathbf{b}| = \tfrac{1}{2}\mathbf{a}\cdot\mathbf{a} \text{ then } \mathbf{a}\cdot\mathbf{c} = 0 \qquad (9.2.2.5e)$$

$$\text{if } (|\mathbf{b}\cdot\mathbf{c}| + |\mathbf{a}\cdot\mathbf{c}| + |\mathbf{a}\cdot\mathbf{b}|) = \tfrac{1}{2}(\mathbf{a}\cdot\mathbf{a} + \mathbf{b}\cdot\mathbf{b}) \text{ then } \mathbf{a}\cdot\mathbf{a} \le 2|\mathbf{a}\cdot\mathbf{c}| + |\mathbf{a}\cdot\mathbf{b}|. \qquad (9.2.2.5f)$$

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.

9.2.3. Main conditions

The main conditions† express the following two requirements:

(i) Of all lattice vectors, none is shorter than $\mathbf{a}$; of those not directed along $\mathbf{a}$, none is shorter than $\mathbf{b}$; of those not lying in the $\mathbf{ab}$ plane, none is shorter than $\mathbf{c}$. This requirement is expressed analytically by (9.2.2.2*a*), and for type-II cells by (9.2.2.4*b*), which for type-I cells is redundant.

(ii) The three angles between basis vectors are either all acute or all non-acute, conditions (9.2.2.2*b*) and (9.2.2.4*c*). As shown in Section 9.2.2 for a given unit cell, the origin corner can always be

† 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 (9.2.2.2*a*)–(9.2.2.5*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 (9.2.2.2*a*)–(9.2.2.5*e*); only (9.2.2.5*f*) is altered. For further details, see Chapter 9.3.

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references