9.3. Further properties of lattices

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9.3.1. Further kinds of reduced cells

In Section 9.2.2, a 'reduced basis' of a lattice is defined which permits a unique representation of this lattice. It was introduced into crystallography by Niggli (1928) and incorporated into *International Tables for X-ray Crystallography* (1969), Vol. I. Originating from algebra (Eisenstein, 1851), a reduced basis is defined in a rather complicated manner [conditions (9.2.2.2*a*) to (9.2.2.5*f*) in Section 9.2.2] and lacks any geometrical meaning. A cell spanned by a reduced basis is called the *Niggli cell*.

However, unique primitive cells may be introduced also in other ways that – unlike the Niggli cell* – have significant geometrical features based mainly on extremal principles (Gruber, 1989). We shall describe some of them below.

If a (primitive) cell of the lattice L fulfils the condition

$$a + b + c = \min$$

on the set of all primitive cells of L, we call it a *Buerger cell*. This cell need not be unique with regard to its shape in the lattice. There exist lattices with 1, 2, 3, 4 and 5 (but not more) Buerger cells differing in shape. The uniqueness can be achieved by various additional conditions. In this way, we can arrive at the following four reduced cells:

(i) the Buerger cell with minimum surface;†
(ii) the Buerger cell with maximum surface;
(iii) the Buerger cell with minimum deviation;‡
(iv) the Buerger cell with maximum deviation.

Equivalent definitions can be obtained by replacing the term 'surface' in (i) and (ii) by the expression

$$\sin\alpha + \sin\beta + \sin\gamma$$

or

$$\sin\alpha \sin\beta \sin\gamma,$$

and by replacing the 'deviation' in (iii) and (iv) by

$$|\cos\alpha| + |\cos\beta| + |\cos\gamma|$$

or

$$|\cos\alpha \cos\beta \cos\gamma|.$$

A Buerger cell can agree with more than one of the definitions

$$\text{(i), (ii), (iii), (iv).} \qquad (9.3.1.1)$$

For example, if a lattice has only one Buerger cell, then this cell agrees with all the definitions in (9.3.1.1). However, there exist also Buerger cells that are in agreement with none of them. Thus, the definitions (9.3.1.1) do not imply a partition of Buerger cells into classes.

It appears that case (iv) coincides with the Niggli cell. This is important because this cell can now be defined by a simple geometrical property instead of a complicated system of conditions.

Further reduced cells can be obtained by applying the definitions (9.3.1.1) to the reciprocal lattice. Then, to a Buerger cell in the reciprocal lattice, there corresponds a primitive cell with absolute minimum surface§ in the direct lattice.

The reduced cells according to the definitions (9.3.1.1) can be recognized by means of a table and found in the lattice by means of algorithms. Detailed mutual relationships between them have been ascertained.

* See, however, later parts of this section.
† Meaning that this cell has the smallest surface of all Buerger cells of the lattice.
‡ The deviation of a cell is the number $|90^\circ - \alpha| + |90^\circ - \beta| + |90^\circ - \gamma|$.
§ This cell need not be a Buerger cell.

9.3.2. Topological characteristic of lattice characters

In his thorough analysis of lattice characters, de Wolff (1988) remarks that so far they have not been defined as clearly as the Bravais types and that an exact general definition does not exist. Gruber (1992) tried to base such a definition on topological concepts.

The crucial notion is the decomposition of a set $\boldsymbol{M}$ of points of the n-dimensional Euclidean space E_n into equivalence classes called *components* of the set $\boldsymbol{M}$. They can be defined as follows: Two points X, Y of the set $\boldsymbol{M}$ belong to the same component if they can be connected by a *continuous* path which lies entirely in the set $\boldsymbol{M}$ (Fig. 9.3.2.1). This partition of the set $\boldsymbol{M}$ into components is unique and is determined solely by the set $\boldsymbol{M}$.

Now let us return to lattices. To any lattice L there is attached a point in E_5 called the *Niggli point* of L. It is the point

$$\left[\frac{\mathbf{a}\cdot\mathbf{a}}{\mathbf{c}\cdot\mathbf{c}}, \frac{\mathbf{b}\cdot\mathbf{b}}{\mathbf{c}\cdot\mathbf{c}}, \frac{2\mathbf{b}\cdot\mathbf{c}}{\mathbf{c}\cdot\mathbf{c}}, \frac{2\mathbf{a}\cdot\mathbf{c}}{\mathbf{c}\cdot\mathbf{c}}, \frac{2\mathbf{a}\cdot\mathbf{b}}{\mathbf{c}\cdot\mathbf{c}}\right] \qquad (9.3.2.1)$$

provided that the vectors **a**, **b**, **c** describe the Niggli cell of L and fulfil the conditions (9.2.2.2*a*) to (9.2.2.5*f*) of Section 9.2.2. If $\mathscr{L}$ is a set of lattices then the set of Niggli points of all lattices of $\mathscr{L}$ is called the *Niggli image* of $\mathscr{L}$.

Thus we can speak about the Niggli image of a Bravais type $\mathscr{T}$. This Niggli image is a part of E_5 and so can be partitioned into components. This division of Niggli points induces back a division of lattices of the Bravais type $\mathscr{T}$. It turns out that this division is identical with the division of $\mathscr{T}$ into lattice characters as introduced in Section 9.2.5. This fact, used conversely, can be considered an exact definition of the lattice characters: Two lattices of Bravais type $\mathscr{T}$ are said to be of the same lattice character if their Niggli points lie in the same component of the Niggli image of $\mathscr{T}$.

We can, of course, also speak about Niggli images of particular lattice characters. According to their definition, these images are connected sets. However, much more can be stated about them: these sets are even *convex* (Fig. 9.3.2.2). This means that any two points of the Niggli image of a lattice character can be connected by a *straight segment* lying totally in this Niggli image. From this property, it follows that the lattice characters may be defined also in the following equivalent way:

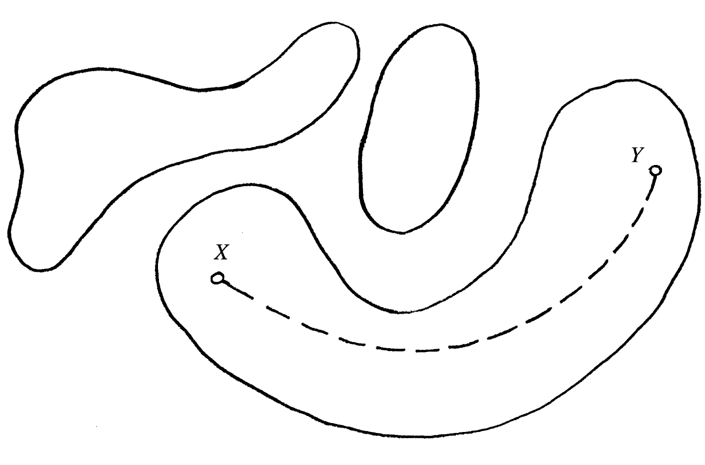

Fig. 9.3.2.1. A set $M \subset E_2$ consisting of three components.

references