

9.3. FURTHER PROPERTIES OF LATTICES

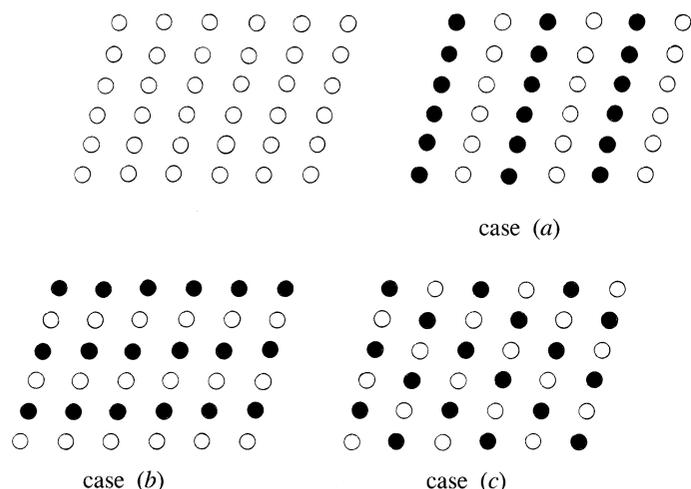


Fig. 9.3.6.1. Three possible decompositions of a two-dimensional lattice L into sublattices of index 2.

L causes a decomposition of the set L into, say, i mutually congruent sublattices, L' itself being one of them (Fig. 9.3.6.1). The number i is called the *index* of the sublattice L' and indicates how many times L' is 'diluted' with respect to L .

Sublattices are defined in a natural way in those lattices that have centred conventional cells, being generated by the vertices of these cells ('decentring'). They are primitive and belong to the same crystal family as the given lattice. Thus, in the cI , cF , tI , oI , oF , oC , mC and hR * lattices, we can meet sublattices of indices 2, 4, 2, 2, 4, 2, 2 and 3, respectively.

Theoretically (though hardly in crystallographic practice), the Bravais type of centred lattices can also be determined by testing all their sublattices with the suspected index and finding in any of these sublattices the Niggli cell.

All sublattices of index i of an n -dimensional lattice L can be constructed by a procedure suggested by Cassels (1971). If $\mathbf{a}_1, \dots, \mathbf{a}_n$ is a primitive basis of the lattice L then primitive bases $\mathbf{a}'_1, \dots, \mathbf{a}'_n$ of all sublattices of index i of the lattice L can be found

by the relations

$$[\mathbf{a}'_1, \dots, \mathbf{a}'_n] = [\mathbf{a}_1, \dots, \mathbf{a}_n] \mathbf{R}^T,$$

where the matrix $\mathbf{R} = [r_{ij}]$ fulfils

$$\begin{aligned} 0 &= r_{ij} && \text{for } 1 \leq i < j \leq n, \\ 0 &\leq r_{ij} < r_{jj} && \text{for } 1 \leq j < i \leq n, \\ r_{11} \dots r_{nn} &= i. \end{aligned} \tag{9.3.6.1}$$

The number $D_{n,i}$ of these matrices is equal to the number of decompositions of an n -dimensional lattice L into sublattices of index i . To determine this number, it is not necessary to construct explicitly the matrices fulfilling (9.3.6.1). The following formulae (Gruber, 1997b) can be used:

(i) If $i = p^q$, where $p > 1$ is a prime number, then

$$D_{n,i} = \underbrace{\frac{p^n - 1}{p - 1} \times \frac{p^{n+1} - 1}{p^2 - 1} \times \frac{p^{n+2} - 1}{p^3 - 1} \times \dots}_{q \text{ times}}$$

(ii) If $i = p_1^{q_1} \dots p_m^{q_m}$ (p_1, \dots, p_m mutually different prime numbers, $m > 1$), we deal with any factor $p_j^{q_j}$ ($j = 1, \dots, m$) according to point (i) and multiply all these numbers to obtain the number $D_{n,i}$.

For example, for $n = 3$ and $i = 2, 3, 4$ and 6 , we obtain for $D_{n,i}$ the values 7, 13, 35 and 91, respectively.

In all considerations so far, the symmetry of the lattice L was irrelevant. We took L simply as a set of points and its sublattices as its subsets. (Thus, for illustrating sublattices, the 'triclinic' lattices are most apt; cf. 'derivative lattices' in Chapter 13.2.)

However, this is not exactly the crystallographic point of view. If, for example, the mesh of the lattice L in Fig. 9.3.6.1 were a square, the sublattices in cases (a) and (b) would have the same symmetry (though being different subsets of L) and therefore would be considered by crystallographers as one case only. The number $D_{n,i}$ would be reduced. From this aspect, the problem is treated in Chapter 13.1 in group-theoretical terms which are more suitable for this purpose than the set-theory language used here.

* When choosing their hexagonal description.