

## 3. ADVANCED TOPICS ON SPACE-GROUP SYMMETRY

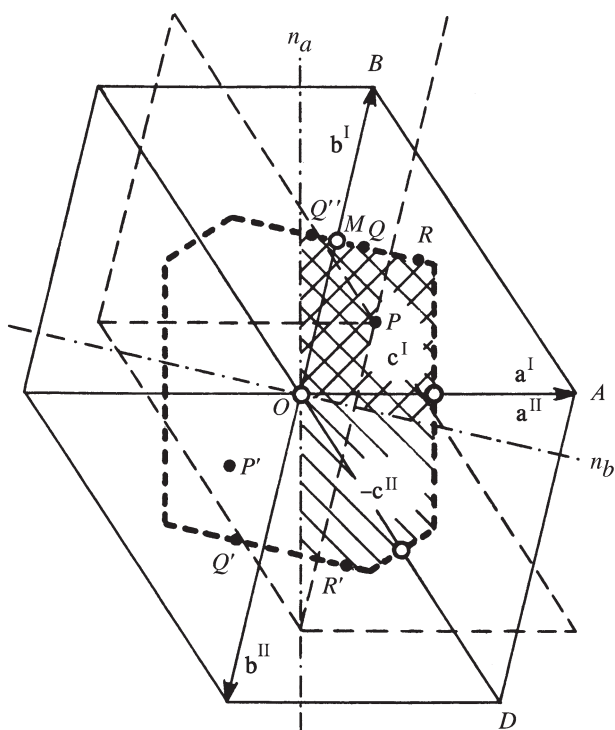


Figure 3.1.3.1

The net of lattice points in the plane of the reduced basis vectors  $\mathbf{a}$  and  $\mathbf{b}$ ;  $OBAD$  is a primitive mesh. The actual choice of  $\mathbf{a}$  and  $\mathbf{b}$  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  $-c^{\text{II}}$  (hatched), the reduced type-II basis is formed by  $\mathbf{a}^{\text{II}}$ ,  $\mathbf{b}^{\text{II}}$  and  $\mathbf{c} = -\overrightarrow{OP}_0$ . Regions marked  $c^{\text{I}}$  (cross-hatched) have the reduced type-I basis  $\mathbf{a}^{\text{I}}$ ,  $\mathbf{b}^{\text{I}}$  and  $\mathbf{c} = +\overrightarrow{OP}_0$ . Small circles in  $O$ ,  $M$  etc. indicate twofold rotation points lying on the region borders (see text).

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  $60 \leq \alpha, \beta, \gamma \leq 120^\circ$ . 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  $\mathbf{a}$ ,  $\mathbf{b}$  and  $\mathbf{c}$  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  $\mathbf{a}$  and  $\mathbf{b}$ , 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  $\mathbf{b}$

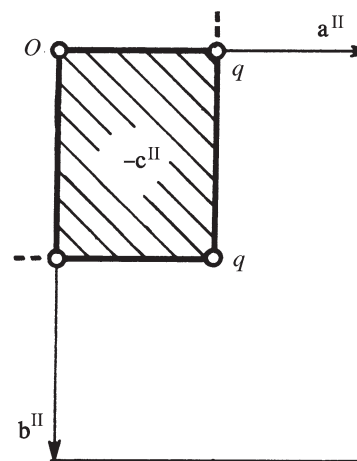


Figure 3.1.3.2

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.  $\mathbf{a}$ ,  $\mathbf{b}$  net primitive orthogonal; special conditions (3.1.3.5c), (3.1.3.5d).

and  $\mathbf{c}$  whenever either (3.1.3.3b) or (3.1.3.5b) is not fulfilled. All the other conditions can be conveniently illustrated by projections of part of the lattice onto the  $\mathbf{ab}$  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  $\mathbf{ab}$  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  $\overline{P}$ , 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  $\mathbf{ab}$  plane is most often (see above) correctly established by (i), the vectors  $\mathbf{a}$ ,  $\mathbf{b}$  and  $\mathbf{c}$  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 (3.1.3.4b); the other edges from (3.1.3.2a). If the spacing  $d$  between  $\mathbf{ab}$  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  $180^\circ$  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