9.1. Bases, lattices, Bravais lattices and other classifications

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9.1.1. Description and transformation of bases

In three dimensions, a coordinate system is defined by an origin and a basis consisting of three non-coplanar vectors. The lengths a, b, c of the basis vectors **a**, **b**, **c** and the intervector angles $\alpha = \angle(\mathbf{b},\mathbf{c})$, $\beta = \angle(\mathbf{c},\mathbf{a})$, $\gamma = \angle(\mathbf{a},\mathbf{b})$ are called the *metric parameters*. In n dimensions, the lengths are designated a_i and the angles α_{ik}, where $1 \le i < k \le n$.

Another description of the basis consists of the scalar products of all pairs of basis vectors. The set of these scalar products obeys the rules of covariant tensors of the second rank (see Section 5.1.3). The scalar products may be written in the form of a (3×3) matrix

$$(\mathbf{a}_i \cdot \mathbf{a}_k) = (g_{ik}) = \mathbf{G}; \quad i,k = 1,2,3,$$

which is called the *matrix of the metric coefficients* or the *metric tensor*.

The change from one basis to another is described by a transformation matrix $\boldsymbol{P}$. The transformation of the old basis (**a**, **b**, **c**) to the new basis $(\mathbf{a}',\mathbf{b}',\mathbf{c}')$ is given by

$$(\mathbf{a}',\mathbf{b}',\mathbf{c}') = (\mathbf{a},\mathbf{b},\mathbf{c}) \cdot \boldsymbol{P}.$$

The relation

$$\mathbf{G}' = \boldsymbol{P}^t \cdot \mathbf{G} \cdot \boldsymbol{P} \qquad (9.1.1.1)$$

holds for the metric tensors **G** and **G**′.

9.1.2. Lattices

A three-dimensional lattice can be visualized best as an infinite periodic array of points, which are the termini of the vectors

$$\mathbf{l}_{uvw} = u\mathbf{a} + v\mathbf{b} + w\mathbf{c}, \quad u,v,w \text{ all integers.}$$

The parallelepiped determined by the basis vectors **a**, **b**, **c** is called a (primitive) *unit cell* of the lattice (*cf.* Section 8.1.4), **a**, **b** and **c** are a primitive *basis of the lattice*. The number of possible lattice bases is infinite.

For the investigation of the properties of lattices, appropriate bases are required. In order to select suitable bases (see below), transformations may be necessary (Section 5.1.3). Of the several properties of lattices, only symmetry and some topological aspects are considered in this chapter. Some further properties of lattices are given in Chapter 9.3.

9.1.3. Topological properties of lattices

The treatment of the topological properties is restricted here to the consideration of the neighbourhood of a lattice point. For this purpose, the *domain of influence* (*Wirkungsbereich*, Dirichlet domain, Voronoi domain, Wigner–Seitz cell) (Delaunay, 1933) is introduced. The domain of a particular lattice point consists of all points in space that are closer to this lattice point than to any other lattice point or at most equidistant to it. To construct the domain, the selected lattice point is connected to all other lattice points. The set of planes perpendicular to these connecting lines and passing through their midpoints contains the boundary planes of the domain of influence, which is thus a convex polyhedron. (Niggli and Delaunay used the term 'domain of influence' for the interior of the convex polyhedron only.) Without the use of metrical properties, Minkowski (1897) proved that the maximal number of boundary planes resulting from this construction is equal to $2(2^n - 1)$, where n is the dimension of the space. The minimal number of boundary planes is $2n$. Each face of the polyhedron represents a lattice vector. Thus, the topological, metrical and symmetry properties of infinite lattices can be discussed with the aid of a finite polyhedron, namely the domain of influence (*cf.* Burzlaff & Zimmermann, 1977).

9.1.4. Special bases for lattices

Different procedures are in use to select specific bases of lattices. The reduction procedures employ metrical properties to develop a sequence of basis transformations which lead to a *reduced basis* and *reduced cell* (see Chapter 9.3).

Table 9.1.4.1. *Lattice point-group symmetries*

Two dimensions				
Lattice point group	2	2*mm*	4*mm*	6*mm*
Crystal family*	*m*	*o*	*t*	*h*
	*m*onoclinic (oblique)	*o*rthorhombic (rectangular)	*t*etragonal (square)	*h*exagonal

Three dimensions							
Lattice point group	$C_i \equiv \bar{1}$	$C_{2h} \equiv 2/m$	$D_{2h} \equiv mmm$	$D_{4h} \equiv 4/mmm$	$D_{3d} \equiv \bar{3}m$	$D_{6h} \equiv 6/mmm$	$O_h \equiv m\bar{3}m$
Crystal family*	*a*	*m*	*o*	*t*	*h*		*c*
	*a*northic (triclinic)	*m*onoclinic	*o*rthorhombic	*t*etragonal	*h*exagonal		*c*ubic

* The symbols for crystal families were adopted by the International Union of Crystallography in 1985; *cf.* de Wolff *et al.* (1985).

references