International Tables for Crystallography (2006). Vol. A, Section 8.2.4, p. 728.

lattices: see Section 8.2.5. Even though the consideration of finite integral-matrix groups in connection with space groups is not common in practical crystallography, these matrix groups play a very important role in the classifications discussed in subsequent sections. Finite integral-matrix groups have the advantage of being particularly suitable for computer calculations.

8.2.4. Geometric crystal classes

The widely used term 'crystal class' corresponds to the 'geometric crystal class' described in this section, and must be distinguished from the 'arithmetic' crystal class, introduced in Section 8.2.3. Geometric crystal classes classify the space groups *and* their point groups, *i.e.* the symmetry groups of the external shape of macroscopic crystals. Classification by morphological symmetry was done long before space groups were known. In Section 8.1.6, the reasons are stated why the two seemingly different classifications agree, namely that of space groups according to their matrix groups $\{\boldsymbol{W}\}$, and that of macroscopic crystals according to the 'point groups' of their sets of face normals.

To define geometric crystal classes, we again compare the matrix parts of the space groups.

Definition: All space groups belong to the same *geometric crystal class* for which the matrix parts are identical if suitable bases are chosen, irrespective of their column parts.

In contrast to the definition of arithmetic crystal classes, nonprimitive bases are admitted. To express this definition in matrix terms, we refer to equation (8.2.3.2) of the previous section.

Definition: Two space groups belong to the same *geometric crystal class* or *crystal class* if there is a *real* matrix $\boldsymbol{P}$ such that

$$\{\boldsymbol{W}'\} = \{\boldsymbol{P}^{-1}\boldsymbol{W}\boldsymbol{P}\} \qquad (8.2.4.1)$$

holds.

In contrast to arithmetic crystal classes where $\boldsymbol{P}$ is a *unimodular integral* matrix, for geometric crystal classes only a *real* matrix $\boldsymbol{P}$ is required. Thus, the restriction $\det(\boldsymbol{P}) = \pm 1$ is no longer necessary, $\det(\boldsymbol{P})$ may have any value except zero.

Example

Referred to appropriate primitive bases, the matrix parts of mirror and glide reflections in space groups *Pm* and *Cm* are

$$\boldsymbol{W}_1 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \bar{1} & 0 \\ 0 & 0 & 1 \end{pmatrix} \text{ and } \boldsymbol{W}_2 = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix},$$

respectively. There is no integral matrix $\boldsymbol{P}$ with $\det(\boldsymbol{P}) = \pm 1$ for which equation (8.2.3.2) holds because $\det(\boldsymbol{P}) = 2(P_{11}P_{22}P_{33} - P_{31}P_{22}P_{13})$.

Thus, *Pm* and *Cm* are members of different arithmetic crystal classes. The matrix

$$\boldsymbol{P} = \begin{pmatrix} 1 & 1 & 0 \\ \bar{1} & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \text{ with } \det(\boldsymbol{P}) = 2,$$

however, does solve equation (8.2.4.1) and, therefore, *Pm* and *Cm* are members of the same geometric crystal class, as are *Pc* and *Cc*.

Clearly, space groups of the same arithmetic crystal class always obey condition (8.2.4.1). Thus, the geometric crystal classes form a classification not only of space groups and space-group types but also of arithmetic crystal classes. There are ten geometric crystal classes in E^2 and 32 geometric crystal classes in E^3; see Fig. 8.2.1.1. As $\{(\boldsymbol{W})\}$ is a matrix representation of the point group of a space group, the definition may be restated as follows:

Definition: Two space groups $\mathcal{G}$ and $\mathcal{G}'$ belong to the same geometric crystal class if the matrix representations $\{\boldsymbol{W}\}$ and $\{\boldsymbol{W}'\}$ of their point groups are equivalent, *i.e.* if there is a real matrix $\boldsymbol{P}$ such that equation (8.2.4.1) holds.

This definition may also be used to classify point groups, *via* their matrix groups, into *geometric crystal classes of point groups*. Moreover, the geometric crystal classes provide a classification of the finite groups of integral matrices. Again, matrix groups of the same arithmetic crystal class always belong to the same geometric crystal class.

Enantiomorphism of geometric crystal classes may occur in dimensions greater than three, as it does for arithmetic crystal classes.

8.2.5. Bravais classes of matrices and Bravais types of lattices (*lattice types*)

Every space group $\mathcal{G}$ has a vector lattice $\mathbf{L}$ of translation vectors. The elements of the point group $\mathcal{P}$ of $\mathcal{G}$ are symmetry operations of $\mathbf{L}$. The lattice $\mathbf{L}$ of $\mathcal{G}$, however, may have additional symmetry in comparison with $\mathcal{P}$.

The symmetry of a vector lattice $\mathbf{L}$ is its point group according to the following definition:

Definition: The group $\mathcal{D}$ of *all* linear mappings which map a vector lattice $\mathbf{L}$ onto itself is called the *point group* or the *point symmetry of the lattice* $\mathbf{L}$. Those geometric crystal classes to which point symmetries of lattices belong are called *holohedries*.

The inversion $\mathbf{x} \rightarrow -\mathbf{x}$ is always a symmetry operation of $\mathbf{L}$, even if $\mathcal{G}$ does not contain inversions. If, for instance, $\mathcal{G}$ belongs to space-group type $P6_3mc$, its point group $\mathcal{P}$ is $6mm$ but the point symmetry $\mathcal{D}$ of $\mathbf{L}$ is $6/mmm$. Thus, the point group $\mathcal{D}$ of the lattice $\mathbf{L}$ is of higher order than the point group $\mathcal{P}$ of $\mathcal{G}$.

Other symmetry operations of $\mathbf{L}$ may also have no counterpart in $\mathcal{G}$. Space groups of type $P6_3/m$, for instance, have inversions but no reflections across 'vertical' mirror planes. The point symmetry of their lattices again is $6/mmm$, *i.e.* in this case too there are more elements in the point group $\mathcal{D}$ of $\mathbf{L}$ than in the point group $\mathcal{P}$ of $\mathcal{G}$.

For purposes of classification, lattices $\mathbf{L}$ will now be considered independently of their space groups $\mathcal{G}$. Associated with each vector lattice $\mathbf{L}$ is a finite group $\mathcal{L}$ of $(n \times n)$ integral matrices which describes the point group $\mathcal{D}$ of $\mathbf{L}$ with respect to some primitive basis of $\mathbf{L}$. This matrix group $\mathcal{L}$ is a member of an arithmetic crystal class; *cf.* Section 8.2.3. Thus, there are some arithmetic crystal classes with matrix groups $\mathcal{L}$ of lattices, *e.g.* the arithmetic crystal class $6/mmmP$. Other arithmetic crystal classes, however, are not associated with lattices, like $6/mP$ or $6mmP$. One can distinguish these two cases with the following definition:

Definition: An arithmetic crystal class with matrix groups $\mathcal{L}$ of lattices is called a Bravais arithmetic crystal class or a *Bravais class*.

By this definition, each lattice is associated with a Bravais class. On the other hand, each matrix group of a Bravais class represents the point group of a lattice referred to an appropriate primitive basis. Closer inspection shows that there are five Bravais classes of E^2 and 14 of E^3. With the use of Bravais classes, lattices may be classified using the following definition:

Definition: All those vector lattices belong to the same *Bravais type or lattice type of vector lattices*, for which the matrix groups belong to the same Bravais class.

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