that two such groups are arithmetically equivalent if there is a basis transformation for the reciprocal-vector module, which transforms main reflections into main reflections and satellites into satellites and which transforms one of the matrix groups into the other. The arithmetic classes are determined by the arithmetic equivalence class of the three-dimensional group K_E [*i.e.* by $\Gamma_E(K)$] and by the components of the modulation wavevector with respect to the corresponding reciprocal-lattice basis. This is because the elements ε are fixed by the relation

$$R\mathbf{q} \equiv \varepsilon\mathbf{q} \text{ (modulo reciprocal-lattice vectors of the basic structure).} \quad (9.8.1.22)$$

Note that these $(3+1)$-dimensional equivalence classes are not simply those one obtains in four-dimensional crystallography, as the relation between the higher-dimensional space V_s and the three-dimensional physical space V plays a fundamental role.

The embedded structures in four dimensions have lattice periodicity. So the symmetry groups are four-dimensional space groups, called *superspace groups*. The new name has been introduced because of the privileged role played by the three-dimensional subspace V. A superspace-group element g_s consists of a point-group transformation (R, ε) and a translation $(\mathbf{v}, \Delta)$. The action of such an element on the four-dimensional space is then given by

$$g_s r_s = \{(R, \varepsilon)|(\mathbf{v}, \Delta)\}(\mathbf{r}, t) = (R\mathbf{r} + \mathbf{v}, \varepsilon t + \Delta). \quad (9.8.1.23)$$

It is important to realize that a superspace-group symmetry of an embedded crystal induces three-dimensional transformations leaving the original modulated structure invariant. Corresponding to (9.8.1.23), one obtains the following relations [*cf.* (9.8.1.13)]:

$$\mathbf{u}_{j'}[\mathbf{q}\cdot(\mathbf{n}' + \mathbf{r}_{j'})] = R\mathbf{u}_j[\mathbf{q}\cdot(\mathbf{n} + \mathbf{r}_j) - \varepsilon\Delta] \quad (9.8.1.24)$$

with

$$\mathbf{n}' + \mathbf{r}_{j'} = R(\mathbf{n} + \mathbf{r}_j) + \mathbf{v}.$$

These are purely three-dimensional symmetry relations, but of course not Euclidean ones.

In three-dimensional Euclidean space, the types of space-group transformation are translations, rotations, rotoinversions, reflections, central inversion, screw rotations, and glide planes. Only the latter two transformations have intrinsic non-primitive translations. For superspace groups, the types of transformation are determined by the point-group transformations. By an appropriate choice of the basis in V_s, each of the latter can be brought into the form

$$\begin{pmatrix} \cos\varphi & -\sin\varphi & 0 & 0 \\ \sin\varphi & \cos\varphi & 0 & 0 \\ 0 & 0 & \delta & 0 \\ 0 & 0 & 0 & \varepsilon \end{pmatrix}; \quad \varepsilon, \delta = \pm 1. \quad (9.8.1.25)$$

By a choice of origin, each translational part can be reduced to its intrinsic part, which in combination with the point-group element (R, ε) gives one of the transformations in V indicated above together with the inversion, or the identity, or a shift in V_I. So, for phase inversion (when $\varepsilon = -1$), the intrinsic shift in V_I vanishes. When $\varepsilon = +1$, the intrinsic shift in V_I is given by τ. It will be shown in Subsection 9.8.3.3 that the value of τ is one of

$$0, \frac{1}{2}, \frac{\pm 1}{3}, \frac{\pm 1}{4}, \frac{\pm 1}{6}. \quad (9.8.1.26)$$

Therefore, a superspace-group element can be denoted by a symbol that consists of a symbol for the three-dimensional part following the conventions given in Volume A of *International Tables for Crystallography*, a symbol that determines ε, and one for the corresponding intrinsic internal translation τ.

9.8.1.4.4. *Generalized nomenclature*

In Section 9.8.4, the theory is extended to structures containing d modulations, with $d \geq 1$. In this case, each point-group transformation in internal space is given by R_I and the associated internal translation by the (d-dimensional) vector $\mathbf{v}_I$. Thus,

$$g_s = \{(R, R_I)|(\mathbf{v}, \mathbf{v}_I)\}.$$

The transformations R and R_I are represented by the matrices $\Gamma_E(R)$ and $\Gamma_I(R)$, respectively. In the following discussion, this nomenclature (but with v_I rather than $\mathbf{v}_I$) is sometimes also applied for the $(3+1)$-dimensional case. The usual formulae are obtained by replacing R_I by ε and v_I by Δ.

9.8.1.4.5. *Four-dimensional space groups*

Four-dimensional space groups were obtained in the $(3+1)$-reducible case by Fast & Janssen (1969) and in the general case by Brown, Bülow, Neubüser, Wondratschek & Zassenhaus (1978). The groups were determined on the basis of algorithms developed by Zassenhaus (1948), Janssen, Janner & Ascher (1969), Brown (1969), and Fast & Janssen (1971). In the book by Brown, Bülow, Neubüser, Wondratschek & Zassenhaus, quoted above, a mathematical characterization of the basic crystallographic concepts is given together with corresponding tables for the dimensions one, two, three, and four. One finds there, in particular, a full list of four–dimensional space groups. The list by Fast & Janssen is restricted to space groups with $(3+1)$-reducible point groups. The four-dimensional groups in the work of Brown *et al*. are labelled by numbers. For these same groups, alternative symbols have been developed by Weigel, Phan, Veysseyre and Grebille generalizing the principles of the notation adopted by *International Tables for Crystallography*, Volume A, for the three-dimensional space groups (Weigel, Phan & Veysseyre, 1987; Veysseyre & Weigel, 1989; Grebille, Weigel, Veysseyre & Phan, 1990).

The difference in the listing of four-dimensional crystallographic groups one finds in Brown *et al*. and in Weigel *et al*. with respect to that in the present tables is not simply a matter of notation. In the first place, here only those groups appear that can occur as symmetry groups of one-dimensional incommensurate modulated phases (there are 371 such space groups). Furthermore, as already mentioned, a finer equivalence relation has been considered that reflects the freedom one has in embedding a three-dimensional modulated structure in a four-dimensional Euclidean space. Instead of 371, one then obtains 775 inequivalent groups for which the name superspace group has been introduced. A $(3+1)$-dimensional superspace group is thus a four-dimensional space group having some additional properties. In Section 9.8.4, the precise definitions are given.

In the commensurate one-dimensionally modulated case, 3833 four-dimensional space groups may occur, out of which 320 already belong to the previous 371. The corresponding additional $(3+1)$-dimensional superspace groups are also present in the listing by Fast & Janssen (1969) and have been considered again (and applied to structure determination) by van Smaalen (1987). The Bravais classes for the commensurate $(3+1)$-dimensional case are given in Table 9.8.3.2(*b*).

The relation between modulated crystals and the superspace groups is treated in a textbook by Opechowski (1986). That between the superspace-group symbols of the present tables and those of Weigel *et al*. is discussed in Grebille *et al*. (1990).

references