Appendix 1

Contracted Twins

The individuals of a cell-twinned module of a crystal structure are related to each other in a way which can not be defined for those of macroscopic twinned crystals. Suppose A and B are individuals of a cell-twinned module. Then, for every atom a_j in A, we find in B an atom b_j related to a_j by cell-twin operation. These pairs of atoms are evidently equivalent in the structure, whether the operation is one of the space group operations or such a one characteristic of space groupoids (Sadanaga, 1963). If a stress is laid on such a one-to-one correspondence of atoms between A and B, the cell-twin operation may be rephrased to be a one-to-one mapping in the theory of groups. This situation is expressed as shown below.

Let $X = x_1, x_2, ..., x_n$ and $Y = y_1, y_2, ..., y_n$ be a pair of point sets. Define one-to-one mapping

$$f\colon\ X \rightarrow Y \tag{1}$$

as $f(X_i) = Y_i,\ i = 1, ..., n.$

The mapping f may be called a cell-twin operation from X to Y. One of the pair of slabs in an (n, n) structure of the lillianite homologues, for example, is then the result of a mapping of the other.

Now, consider an idealized model for an (n, n') structure of the lillianite homologues (Fig. 16a of Chapter 3). We then note that complete one-to-one correspondence no longer exists but it is restricted to between a subset of atoms in one slab and whole set of atoms in the other. Such a situation can be expressed by a contracted mapping. Namely, let $X' \subset X$ and $Y = f(X')$. Then the mapping is given in the form:

$$f|X'\colon\ X' \rightarrow Y. \tag{2}$$

By analogy of the case of (1), the mapping (2) may be called a contracted twin-operation. Any composite of structure modules which is characterized by such a contracted mapping may then be called a '*contracted twin*'.

In real (n, n') structures, however, positional correspondence of atoms between slabs exists only approximately owing to distortion of structures from their idealized forms. Nevertheless, the above definition of contracted twin may be extended to apply to describing those real (n, n') structures. In view of the fact that quite a few phases have been known to have the (n, n') structure types as discussed in Chapter 3 and Chapter 4 (see also Andersson and Hyde, 1974), it is thought to be worthwhile to introduce such a terminology.

REFERENCE

Andersson, S. and Hyde, B. G. (1974): vid. Chapter 3.
Sadanaga, R. (1963): vid. Summary and Comments.