Examination of Space-Groupoid Theory

I. Theory of Sadanaga and Ohsumi

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Abstract

Theories of space-groupoids and of vector symmetry of Sadanaga & Ohsumi [*Acta Cryst.* (1979), **A35**, 115-122] are analyzed by means of ordinary space-group theoretical method. The space-groupoids by their representation are proved to be empty sets. The three space-groupoid structures exemplified by them are not space-groupoid structures except one of them. The space-groupoid theory is concluded to be not necessary for crystallography. The first theorem of vector symmetry proposed by them is proved to be tautology by analyzing the concept of self-homometry, which is interpreted to be synonymous with homometry. The second theorem of vector symmetry is pointed out to be wrongly formulated and groundless.

1. Introduction

Crystal structures giving rise extraordinary extinctions of diffracted spectra or diffuse streaked spectra were called OD-structures by Dornberger-Schiff (1956). In order to describe symmetries of such structures, Dornberger-Schiff & Grell-Nieman (1961) introduced groupoids of Brandt (1927) and formulated space-groupoid theory. OD-structures and space-groupoid theory were discussed by Dornberger-Schiff (1964) in detail. Since one of the subjects for the present author's study is calculation of X-ray diffracted intensity by close-packed structures with stacking faults, the author have recognized that OD-structure theory is useless for the calculation. The extraordinary extinctions can be interpreted by ordinary space-group theoretical method and the space-groupoid theoretical interpretation is nothing but confusion.

Space-groupoid theory was assented by Sadanaga and his school in Japan. They applied the theory to enhancement of diffraction symmetry. The enhancement of diffraction symmetry means that the point group of a diffraction pattern is of higher order than that generated by the point group of the crystal and an inversion operation. The point group of a diffraction pattern agrees with the point group of the vector set, where a vector set means the set of vectors directed from the positions of atoms to those of

the other atoms in a crystal. Sadanaga & Ohsumi (1979) discussed symmetries of vector sets as if they showed one of applications of space-groupoid theory, and formulated two theorems for symmetries of vector sets, for which they insisted to be useful to interpret the enhancement of diffraction symmetry.

The structures discussed by Sadanaga & Ohsumi(1979) have translation symmetry and are more adequate than OD-structures for application of the groupoid theory. However, we find out at glance very strange facts in the examples given by them. In a structure consisting of three substructures with the same lattice, any one of which is said to be obtained by a space-groupoid operation on another substructure. There are squares with different lengths of sides which are said to be space-groupoid symmetric with each other. These space-groupoid operations are not compatible with the lattice translation symmetry. In another example, they insisted that there were operations bringing a kind of atoms to another kind of atoms. They described that a space group could be transformed to another inequivalent one. These space-groupoid operations contradict the fundamentals of crystallography. If introduction of these kinds of operations into crystallography are allowed, crystallography will be destroyed. In this paper, the present author deduces many strange operations which can not be compatible with space group theory.

We can discuss the symmetry of a vector set by using space group theoretical method. The theory of symmetries of vector sets of Sadanaga & Ohsumi (1979) is based on misunderstanding of homometry. Their important concept "self-homometry" is shown to be nothing but identity if we interpret literally the description of them. In order to analyze their theory, the present author makes clear that self-homometry should be interpreted to be homometry. Many undefined terms used inconsistently by them are defined clearly. The first theorem of vector symmetry of them is shown to be tautology. A method to obtain counter-examples of the second theorem is described and a counter-example is shown in this paper. Theorems for necessary conditions become false if a counter-example is found. Hence, the second theorem is false.

Sadanaga & Ohsumi (1979) will be refered to S-O, hereafter.

2. Space-groupoids

Crystals are characterized to have translation symmetry, see Seitz (1935). Translation symmety means that a crystal is brought onto itself by translations which are expressed by vectors $n_1\boldsymbol{a}+n_2\boldsymbol{b}+n_3\boldsymbol{c}$, where $\boldsymbol{a}$, $\boldsymbol{b}$ and $\boldsymbol{c}$ are the bases of the translations

and for n_i any integers, see Appendix A. When we express points in space by the position vectors, the set of the points

$$\boldsymbol{T}=\{n_1\boldsymbol{a}+n_2\boldsymbol{b}+n_3\boldsymbol{c};\ \text{for } n_i \text{ any integers}\} \tag{1}$$

is called point-lattice, see Burckhardt (1966), and the set $\boldsymbol{T}$ as that of the translation vectors is called lattice. Translation symmetry means as follows, if there is a atom at $\boldsymbol{r}$, there are the same kind of atoms at the positions, $\boldsymbol{r}'$,

$$\boldsymbol{r}'=\boldsymbol{r}+n_1\boldsymbol{a}+n_2\boldsymbol{b}+n_3\boldsymbol{c};\qquad \text{for } n_i \text{ any integers.} \tag{2}$$

The set of the equivalent positions of the atom is expressed by

$$(\boldsymbol{r}+\boldsymbol{T})=\{\boldsymbol{r}+n_1\boldsymbol{a}+n_2\boldsymbol{b}+n_3\boldsymbol{c};\ \text{for } n_i \text{ any integers}\}. \tag{3}$$

Symmetry operations defined by Brown, Bülow, Neubüser, Wondratschek and Zassenhaus (1978) are as follows.

"A symmetry operation of an object in space is mapping of the space onto itself satisfying the following conditions:

1. It is a rigid motion; that is, it leaves all distances unchanged.
2. It maps the object as a whole onto itself; that is, the object after mapping is indistinguishable from the original object.

If the object is a crystal structure, its symmetry operations are called crystallographic symmetry operations."

Since we treat always crystals, crystallographic symmetry operations are called simply symmetry operations. It must be noted that the extension of the object should be infinite and the mapping should be one-to-one in the above definition.

A rigid motion consists of a displacement followed by a rotation, where the rotation means the rotation in wide sense, that is, it may be a reflection, an inversion or an inversion rotation. A rigid motion g operated on a position vector $\boldsymbol{r}$ can be expressed by

$$g\boldsymbol{r}=A\boldsymbol{r}+\boldsymbol{a}, \tag{4}$$

where A is a rotation which is represented by a matrix with determinant ±1 and $\boldsymbol{a}$ is a vector. Seitz (1935) called A and $\boldsymbol{a}$ the rotation matrix and the translation vector, respectively. The motion g is represented by an operator

$$g=(\mathrm{A}, \boldsymbol{a}). \tag{5}$$

A space group G is represented by the following form,

$$G=T(A_1,0)+T(A_2,\boldsymbol{a}_2)+\cdots\cdots \tag{6}$$

where

$$T=\{(E,\boldsymbol{n});\ \boldsymbol{n}\in\boldsymbol{T}\} \tag{7}$$

and $A_1=E$ is a unit operation.

Rotations of a space group G leave the translation group T of G invariant and form one of thirty-two rotation-groups, see Seitz (1935). The set of points obtained by operating all the elements of G on a point at a general position forms a regular point system, see Burckhardt (1966). The set of the position vectors of the points equivalent with a point at $\boldsymbol{r}$ is expressed by

$$\begin{aligned} X(\boldsymbol{r}) &= \{g\boldsymbol{r};\ g\in\boldsymbol{G}\} \\ &= \sum_i((A_i,\boldsymbol{a}_i)\boldsymbol{r}+\boldsymbol{T}). \end{aligned} \tag{8}$$

If the point is at a general position, the set $X(\boldsymbol{r})$ becomes a representation of the regular point system and corresponds to G one-to-one. When the space group G is symmorphic, the set $X(0)$, the set of the position vectors of the equivalent points with the origin of the lattice, agrees with $\boldsymbol{T}$. If we regard the atoms as points, a crystal structure becomes the direct sum of the set $X(\boldsymbol{r}_i)$, where $\boldsymbol{r}_i$ is ith atom's position,

$$\begin{aligned} X &= \sum_i X(\boldsymbol{r}_i) \\ &= \sum_i\sum_j((A_j,\boldsymbol{a}_j)\boldsymbol{r}_i+\boldsymbol{T}). \end{aligned} \tag{9}$$

Since crystal structures can be characterized by the sets Xs of the position vectors, the sets are called also the crystal structures, and a point P of which the position vector is $\boldsymbol{r}$ is called simply the point $\boldsymbol{r}$, hereafter.

Dornberger-Schiff (1956) proposed that structures consisting of a set of equal translatable layers, with successive layers related by one of several stacking vectors $\boldsymbol{s}_i$, which are derived from one another or from the inverse of the other by symmetry elements of single layer should be denoted by the term OD-structures of type A. Dornberger-Schiff & Grell-Nieman (1961) called operations transforming any layer into itself as λ-POs and those transforming a layer into adjacent layer as σ-POs. According to Dornberger-Schiff (1964), the both kinds of operations form a Brandt's groupoid.

S-O applied the groupoid theory to quite a different kind of structures from OD-structures. Their crystal structures are composed of several substructures with the

same lattice. We can not divide such structures into definite domains as done in OD-structures, since any small domain in the structures consists of the domains with the same size of each substructures. According to S-O, such structures have two classes of operations, the one is composed of operations bringing each of the substructures onto itself, and the other is composed of operations bringing each of substructures onto another one. The former class of the operations form a group and the set of operations is called the kernel of the groupoid and is denoted by K_0. The set of the operations belonging to the latter class is called the hull of the groupoid and is denoted by H. The groupoid is expressed by the direct sum of $h_i^{-1}K_0h_j$,

$$M=\sum_{i=0}\sum_{j=0}h_i^{-1}K_0h_j, \tag{10}$$

where $h_i\in H$. In Eq. (10), h_j brings the jth substructure X_j onto the substructure X_0 representing the kernel K_0. From the definition of the kernel, the space groups of all the substructures must be the same as K_0.

Let us investigate the nature of the elements of the hull H. The elements must absolutely not be sets of operations. If the elements are the sets of operations, the space-groupoid M becomes an empty set, since the product of two sets is the intersection of the sets, see Iyanaga and Kawada (1977). The definition that h_i brings the ith substructure X_i onto the 0th substructure X_0 means that h_i is a one-to-one mapping of X_i onto X_0,

$$X_0=\{h_i\boldsymbol{r}';\ \boldsymbol{r}'\in X_i\}. \tag{11}$$

When we assume that X_0 consists of an atom at $\boldsymbol{r}$ and its equivalent ones, X_0 can be expressed by

$$X_0=\{g\boldsymbol{r};\ g\in G\}, \tag{12}$$

where G is the space group of X_0. The substructure X_i is rewritten by

$$X_i=\{h_i^{-1}g\boldsymbol{r};\ g\in G\}. \tag{13}$$

The both substructures have the same lattice. The lattice of which origin at the origin of X_0, $\boldsymbol{T}$, is brought by the operation h_i^{-1} to that of X_i. The origin of the lattice of X_i should be at the origin of X_i which is apart from that of X_0 by $\boldsymbol{b}_i$. That is to say, $h_i^{-1}\boldsymbol{T}$ becomes

$$\begin{aligned} h_i^{-1}\boldsymbol{T} &= \{h_i^{-1}(n_1\boldsymbol{a}+n_2\boldsymbol{b}+n_3\boldsymbol{c});\ \text{for } n_i \text{ any integers}\} \\ &= \{\boldsymbol{b}_i+n_1\boldsymbol{a}+n_2\boldsymbol{b}+n_3\boldsymbol{c};\ \text{for } n_i \text{ any integers}\} \\ &= (\boldsymbol{b}_i+\boldsymbol{T}). \end{aligned} \tag{14}$$

Since the operation h_i^{-1} leaves the distances between the lattice points unchanged, the operation h_i^{-1} must be a rigid motion, which can be represented by the form of

$$h_i^{-1}=(B_i, \boldsymbol{b}_i). \tag{15}$$

The rotation B_i must transform $\boldsymbol{T}$ invariant

$$B_i\boldsymbol{T}=\boldsymbol{T}. \tag{16}$$

The rotation B_i should be an element of the holohedry. Therefore, the elements of hull should be:

> An operation h_i^{-1} of hull is a rigid motion; the rotation of B_i of h_i^{-1} is an element of the holohedry and the translation $\boldsymbol{b}_i$ is the vector from the origin of X_0 to that of X_i.

The reverse element h_i of h_i^{-1} is

$$h_i=(B_i^{-1}, -B_i^{-1}\boldsymbol{b}_i). \tag{17}$$

We can verify that the elements of hull represented by Eqs. (15) and (17) satisfy groupoid's definitions. When $\boldsymbol{r}\in X_0$, the element $\boldsymbol{r}'$ equivalent with $\boldsymbol{r}$ in X_i is $(B_i, \boldsymbol{b}_i)\boldsymbol{r}$. When an element of $h_i^{-1}Mh_i$, represented by

$$(B_i, \boldsymbol{b}_i)k(B_i^{-1}, -B_i^{-1}\boldsymbol{b}_i), \tag{18}$$

is operated on $\boldsymbol{r}'$, we have

$$(B_i, \boldsymbol{b}_i)k(B_i^{-1}, -B_i^{-1}\boldsymbol{b}_i)(B_i, \boldsymbol{b}_i)\boldsymbol{r}=(B_i, \boldsymbol{b}_i)k\boldsymbol{r}\in X_i, \tag{19}$$

and when an element of $h_j^{-1}Mh_i$ is operated on $\boldsymbol{r}$, we have

$$(B_j, \boldsymbol{b}_j)k(B_i^{-1}, -B_i^{-1}\boldsymbol{b}_i)(B_i, \boldsymbol{b}_i)\boldsymbol{r}=(B_j, \boldsymbol{b}_j)k\boldsymbol{r}\in X_j. \tag{20}$$

We can conclude that the space-groupoids are represented by our representations.

Two operations a and b belonging to a space group G are said to be identical if the results of the both operations on any points in a crystal space D agree with one another, that is,

$$ar=br \tag{21}$$

for any points in D, then

$$a=b. \tag{22}$$

If the results are different from one another at one point at least in D, the operation a is said to be not identical with the operation b. If a point does not satisfy Eq. (21) for any two operations belonging to G, the point is said to be at a general position, if the point is not a general position, the point is said to be at a special position. The number of equivalent points with a point at the special position becomes smaller than that of the points at general positions, but the symmetry between the points does not change, see Appendix A.

In the cases of groupoids, eventhough a point r_p satisfies

$$h_0k_s\boldsymbol{r}_P=h_i^{-1}k_t\boldsymbol{r}_P, \tag{23}$$

the set $X_i(\boldsymbol{r}_P)$ does not agree with $X_0(\boldsymbol{r}_P)$, since K_0 is not a normal subgroup of M, $K_0 \neq h_i^{-1}K_0h_i$. In this case, there is one element belonging to $X_0(\boldsymbol{r}_P)$ and not belonging to $X_i(\boldsymbol{r}_P)$ at least, say $\boldsymbol{r}_S$,

$$X_0(\boldsymbol{r}_P)-X_0(\boldsymbol{r}_P)\cap X_i(\boldsymbol{r}_P)\supseteq\{\boldsymbol{r}_S\}. \tag{24}$$

The two points $\boldsymbol{r}_S$ and $\boldsymbol{r}_P$ are at equivalent positions with respect to K_0, the situation of surroundings about the point $\boldsymbol{r}_P$ in the crystal space must be the same as that about $\boldsymbol{r}_S$ in ordinary structures. Hence, the coincidence of $\boldsymbol{r}_P$ with $k_s^{-1}h_i^{-1}k_t\boldsymbol{r}_P$ should be regarded as an accidental coincidence. This interpretation is supported by the fact that the one-to-one correspondence between X and $\sum_i h_i^{-1}K_0$ is lost, if there is a common element in the both sets and the element is not counted doubly.

Structures composed of substructures were discussed by the present author (1977) about the enhancements of diffraction symmetries, the extraordinary extinctions of diffracted spectra, and the conditions for the set $SB=\{(B_i, b_i)\}$ and the space group of the substructures generating a space group. Although the objects of studies are quite the same, the methods explicitly described and the understandings of the structures are quite different from each other. The difference is shown in the following section.

3. Analysises of examples

The examples of space-groupoid structures given by S-O are shown in Figs. 1, 2 and 3. In Fig. 1, the 0th substructure X_0 consists of two white circles and one black one, of which coordinates are;

$$\boldsymbol{r}_1=(x,0,z),\ \boldsymbol{r}_2=(\bar{x},0,\bar{z}) \quad \text{for white circles,}$$
$$\boldsymbol{r}_3=(0,y,0), \quad \text{for black circle.}$$

The vectors $\boldsymbol{b}_1$ and $\boldsymbol{b}_2$ are drawn in Fig. 1. The space group of the substructures is $P2$ and the symmetry between substructures is

$$SB=\{(E,0),(E,\boldsymbol{b}_1),(E,\boldsymbol{b}_2)\}.$$

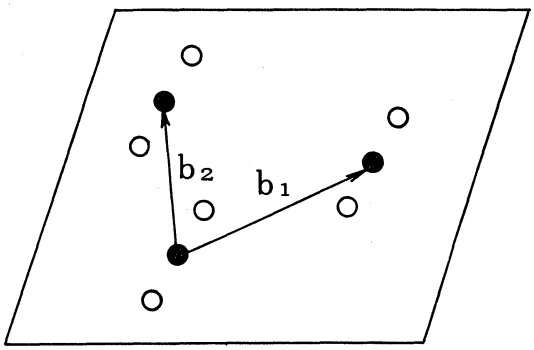

Fig. 1. Fig. 6 of S-O. This structure is only one example of space-groupoid structures, but does not satisfy the second theorem of vector summetry of S-O.

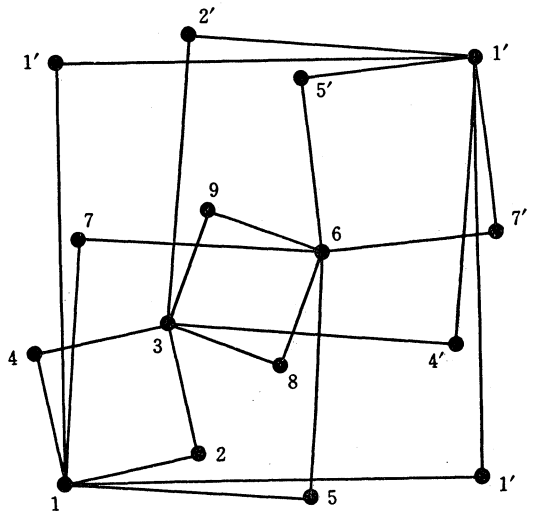

Fig. 2. Fig. 7 of S-O. This structure is not a space-groupoid structure and does not satisfy the second theorem of vector symmetry of S-O.

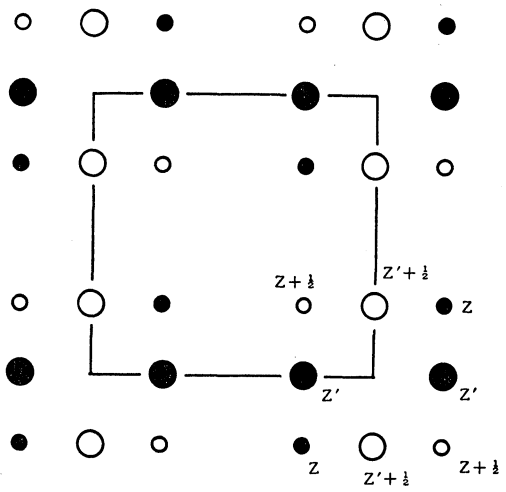

Fig. 3. Fig. 8 of S-O. This structure is also not a space-groupoid structure. This structure is not suitable for the example of the second theorem since the diffraction enhancement occurs owing to the product of the structure factors of the substructures is zero.

The set SB must agree with $\{h_0, h_1^{-1}, h_2^{-1}\}$. In this example, we can not define the subspace where "the local symmetry operations are effective", since the space group $P2$ is effective everywhere for the 0th substructure in the crystal space. This example seems to satisfy the postulations of space-groupoids interpreted by the present author, but the readers should aware that the space-groupoid theory can not deduce any crystallographically useful informations for this structure. We can discuss enhancement of diffraction symmetry very easily from ordinary space group theoretical treatment, see Takahashi (1977).

In Fig. 2, the points are numbered by the present author. The points with dashed numbers are translatively equivalent to those with the undashed same numbers. We denote by (a, b, c, d) a square formed by points a, b, c and d and by $\{a, b, c, d\}$ the substructure formed by the translatively equivalent squares with (a, b, c, d).

We can judge at a glance that there is no rigid motion which maps the square (1, 2, 3, 4) onto the other square, say (1, 5, 6, 7). The operation h_1^{-1} mapping (1, 2, 3, 4) onto (1, 5, 6, 7) is represented by

$$h_1^{-1}=(cR, \boldsymbol{b}_1)$$

where R is the rotation bringing (1, 2, 3, 4) parallel to (1, 5, 6, 7), $\boldsymbol{b}_1$ is the vector from the center of (1, 2, 3, 4) to that of (1, 5, 6, 7), $c=|\boldsymbol{r}_1-\boldsymbol{b}_1|/|\boldsymbol{r}_1|$ and $\boldsymbol{r}_1$ is the vector from center of (1, 2, 3, 4) to the point 1. Since $c \neq 1$, the operation h_1^{-1} changes the distances

between any two points in (1, 2, 3, 4) by the mapping. The rotation R rotates the lattice of {1, 2, 3, 4} by the same angle with which (1, 2, 3, 4) is rotated, and does not make coincidence the substructure {1, 2, 3, 4} with {1, 5, 6, 7}. The rotation varies with the position $\boldsymbol{r}_1$.

According to S-O, the element of the hull transforming the ith substructure X_i to X_0 in Fig. 2 is given by the product of the three factors R_i, U_i and t_i, $h_i=U_i\cdot R_i\cdot t_i$. The factor t_i is "a partial translation which brings the plane lattice L_i composed of the centers of the squares in X_i to superpose upon the corresponding lattice L_0 in X_0". The factor R_i is "a set" and expressed by "$\cup_j T_j r_i T_j^{-1}$, where r_i is a partial rotation operating on the squares in X_0, T_j is a lattice translation from the origin of L_i to the jth lattice point in L_i, and the union ranges over all the lattice points in L_i,". Since R_i is a set, $T_j r_i T_j^{-1}$ must be a subset of R_i. The factor U_i is "a set" and expressed by "$U_i=\cup_j T_j u_i T_j^{-1}$, where u_i is a similarity transformation operating on the above square to make it the same size as the square in X_0." Similarly to the case of R_i, $T_j u_i T_j^{-1}$ must be a subset of U_i.

The present author revises the above S-O's descriptions in accordance with the set theory. The factor t_i can be represented by

$$t_i=(E, -\boldsymbol{b}_i).$$

The factor R_i should not be $\cup_j T_j r_i T_j^{-1}$, but

$$R_i=\{T_j r_i T_j^{-1};\ T_j\in T\}.$$

Since r_i is represented by $(r_i, 0)$, R_i should be represented by

$$R_i=\{(E, \boldsymbol{n})(r_i, 0)(E, -\boldsymbol{n});(E, \boldsymbol{n})\in T\}.$$

The factor U_i should be

$$U_i=\{T_j u_i T_j^{-1};\ T_j\in T\}.$$

Since $u_i=c_i E$, where c_i is a scaling factor, U_i should be

$$U_i=\{(E, \boldsymbol{n})(c_i E, 0)(E, -\boldsymbol{n});\ (E, \boldsymbol{n})\in T\}.$$

Of course, the product $U_i\cdot R_i\cdot t_i$ is an empty set.

According to Loewy (1927), there is no common element between $K_0 h_i$ and $K_0 h_j$ if $h_i \neq h_j$, then there is also no common element between $h_i^{-1}K_0$ and $h_j^{-1}K_0$. Since the points 1 and 3 are equivalent to one another with respect to K_0, if the point 1 is at a

general position, so is the point 3. The points 1 and 6 are equivalent to one another, the point 6 is also at a general position. Since we can put the point 1 everywhere in the unit cell, the position can not belong to two substructures except an accidental coincidence. Since the correspondence between K_0 and $h_i^{-1}K_0$ is one-to-one, the point belonging to one of substructures must correspond uniquely to those of the other substructures, that is, all the substructures must have the same number of points. If there are common points in two substructure, the points must be doubled. According to S-O, all the points in Fig. 2 are of equal weight, and all the squares and translationally equivalent ones form the substructures. This contradicts one-to-one correspondence between X_i and X_j, since all the points have equal weight. If we allow the existence of the common points of equal weight with the other points, we must introduce anihilation and creation operations of atoms into crystallography.

The structure in Fig. 3 is composed of two substructures, one with the symmetry of $P4_2cm$ consisting of small circles, and the other with $P4_2mc$ consisting of large circles. The small and large circles have different weight, that is, they are different kinds of atoms to each other. If we can make map one of the substructures onto the other one, we must be required to introduce the following two kinds of operations;

a. operations changing the distances between two points,

b. rotation by $\pi/4$.

The former kind of operations are not rigid motions and the latter kind of rotation does change the direction of the lattice. In addition, in order that one of the substructures is mapped by the other one, we must introduce operations changing the kinds of atoms. If these operations are allowed, we could make all atoms equivalent in a crystal structure regardless the kinds of atoms. Since one of the substructures can not be mapped onto the other one, the structure does not have the kernel of groupoid, and is not a space-groupoid structure, see Appendix A.

The above examinations show the space-grpoupoid theory of S-O is not necessary for crystallography and should be disregarded by Occam's razor.

4. Self-homometry

A set V of vectors which are directed from atoms to the other atoms in a crystal structure X is called the vector set of X, that is, if

$$X=\{\boldsymbol{r}_i;\ i\leq N\}, \tag{25}$$

then

$$V=\{\boldsymbol{r}_i-\boldsymbol{r}_j;\ \boldsymbol{r}_i, \boldsymbol{r}_j\in X\}. \tag{26}$$

The ordinary definition of homometry is as follows. When the two sets of position vectors are denoted by X_A and X_B and the vector sets by V_A and V_B, respectively, for two structures A and B, if the two structures satisfy the following two conditions

$$X_A \neq X_B \text{ and } X_A \neq \overline{X}_B \tag{27}$$

and

$$V_A=V_B, \tag{28}$$

the two structures are said to be homometric with one another, where $\overline{X}_B$ is the inversion of X_B. In this paper, the author modifies slightly the above definition as follows:

If $X_A \neq X_B$ and $V_A=V_B$, A is homometric with B.

If the structure A is homometric with B, we denote by

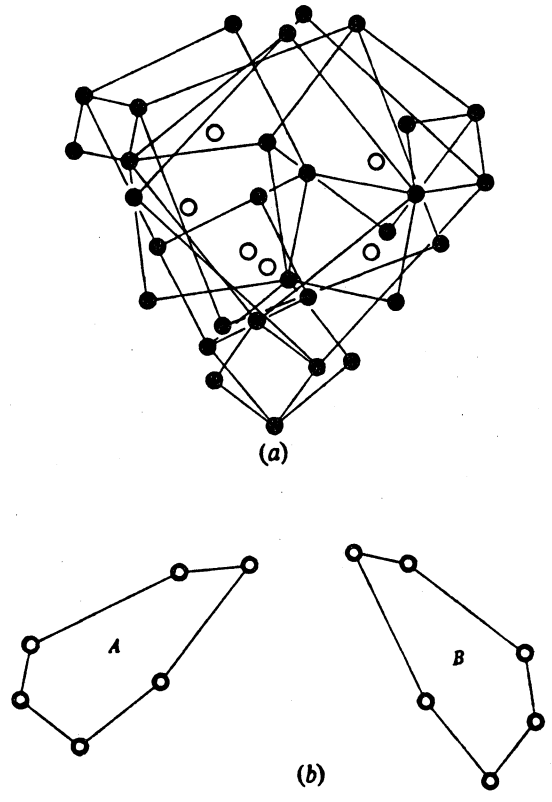

Fig. 4. Fig. 4 of S-O. The point group of the structure (*a*) is 1 and the diffraction symmetry is 4.

$$A \overset{h}{=} B. \tag{29}$$

According to S-O, self-homometry is defined as follows.

"Let us assume that the structure X is homometric with itself in such a way that both A and B, which are homometric with each other, come to coincide with each other with X. The structure X will then be said to be self-homometric."

In the above description, we can not know how the two structures A and B relate with X. By Consulting the example given in Fig. 4, X might be the convolution of A and B,

$$X = A*B. \tag{30}$$

If so, "self-homometry" of S-O may be as follows:

"When a structure X is the convolution of A and B, and A is changed to B by a homometric operation P and B is done to A by P, the operation P is called a self-homometric operation if $PX=PA*PB$ is homometric with X,

$$PX = PA*PB = B*A \overset{h}{=} X." \tag{31}$$

Here the operations changing structures to the other homometric structures are called homometric operations. According to Hosemann & Bagchi (1954), $A*B$ is identical to $B*A$,

$$A*B = B*A. \tag{32}$$

Hence, the self-homometry of S-O is nothing but identity. The author shows that self-homometry of S-O must be homometry by analyzing the example given in Fig. 4. That is, the self-homometry of S-O is based on misunderstanding of homometry.

Although homometric operations can not be found in general, we can find the operations for special cases. For example, when we number the points of A in Fig. 4(b) and form a column matrix of which ith element is $\boldsymbol{r}_i - \boldsymbol{r}_{i+1}$, then we can find a matrix transforming the column matrix to that of B rotated by $-\pi/2$. The transformation matrix P is a representation of the homometric operation. We can examine easily the following relations,

$$P^2 = e \tag{33}$$

and

$$P(A*B) = PA*PB, \tag{34}$$

where e is a unit operation. The product of a rotation R and a homometric operation P is commutative,

$$PR=RP. \tag{35}$$

The structure in Fig. 4(a) is obtained by the convolution of A and $B=RPA$, where R is a rotation by $\pi/2$ and P is a homometric operation on A. The operation transforming A to B is not a homometric operationon on A but a homometric operation followed by the rotation R. If we operate RP on $A*B$, $A*B$ is transformed to a homometric structure with $A*B$, that is,

$$\begin{aligned} RP(A*B) &= RP(A*RPA) \\ &= RPA*\bar{A} \\ &\overset{h}{=} A*RPA \\ &= A*B. \end{aligned} \tag{36}$$

Hence, we recognize that that the definition of S-O for self-homometry is quite meaningless.

We can prove directly that the vector set of $A*B$ has 4-fold rotation symmetry. The structure $A*B$ is transformed by R to a homometric structure,

$$\begin{aligned} R(A*B) &= R(A*RPA) \\ &= RA*P\bar{A} \\ &\overset{h}{=} RPA*A \\ &= A*B. \end{aligned} \tag{37}$$

The vector set V_{A*B} is invariant by the rotation R. Since

$$\begin{aligned} R^3(A*B) &= R(\bar{A}*\bar{B}) \\ &\overset{h}{=} R(A*B) \end{aligned} \tag{38}$$

the vector set V_{A*B} has 4-fold rotation symmetry, see Appendix B.

5. Two theorems of vector symmetry

The concept of self-homometry turns out to be meaningless in the preceding section. The two theorems of vector symmetry of S-O are formulated on the meaningless concept, so that they are evidently valueless. However, in order to show that S-O formulated

them arbitrarily and independently of space-groupoid theory, they are analyzed in this section.

The first theorem of vector symmetry given by S-O is as follows:

"The necessary and sufficient condition for a structure X to be n-fold vector symmetric is that X is n-fold self-homometric."

We can not know what mean "X to be n-fold vector symmetric" and "X is n-fold self-homometric" in the first theorem, since S-O did not define n-fold vector symmetry and n-fold self-homometry. In this section, the terms used by S-O are redefined along the contexts of their usage, regardless the analyses in the preceding section.

The term n-fold self-homometry and its related terms are revealed by analyzing the following sentences. "Conversely, when V is n-fold symmetric, it will be superposed upon itself by a rotation of $2\pi/n$ around its n-fold rotation axis N. This means that X consists of vectors which correspond one-to-one in both equality in length and parallelism in direction to the vectors in X after a rotation by $2\pi/n$ around an axis parallel to N in V, that is, X is n-fold self-homometric." At first, it must be noted that the both axes pass through the origin of the lattice, since all the proper or improper rotations in space groups have the origins of the lattices as the fixed points. The former sentence in the quatation means that V is n-fold rotation symmetric. In the latter sentence, it means that V is also n-fold rotation symmetric, since the vectors in X mean the vectors between atoms in X. Consequently, n-fold self-homometry of X is synonymous with n-fold rotation symmetry of V.

From the above analysis, we can define the terms relating with self-homometry as follows. When we denote by X' the set of position vectors obtained by a rotation R on the set X, $X'=RX$, where the rotation angle is $2\pi/n$, and by V and V' the vector sets of X and X', respectively, we define:

(a) n-fold self-homometry

If $V=V'$, X is n-fold self-homometric.

(b) n-fold vector-symmetry

If $V=V'$, X is n-fold vector-symmetric.

By taking account of the description of S-O that self-homometry includes global symmetry, n-fold self-homometry does not concern with either $X=X'$ or not, so that our definition (a) is ascertained. Vector symmetry of S-O is symmetry in vector set. Symmetry in

vector set also does not concern with either $X=X'$ or not, so that our definition (*b*) is ascertained. The definitions (*a*) and (*b*) accord with the usage of S-O. When global and local symmetries are excluded from self-homometry, the remainder is called proper self-homometry by S-O. That their understanding of homometry is quite wrong is also shown easily if we refer to an ordinary structure having the space group $P3$. This structure can be divided into three substructure which are equivalent with one another, but the vector sets of the substructures are not equal to one another. That is to say, global symmetry is not necessarily self-symmetry in the sense of S-O. Of course, $X=X'$ and $V=V'$ in this case.

The above definitions conclude that the first theorem is tautology. The origin of this tautology is the extension of the wrong concept of self-homometry to ordinary symmetry. Self-homometry is defined for the structures obtained by the convolution of two structures and not defined for the other kinds of structures. Neverthless, S-O extended the concept to even ordinary symmetry which governs ordinary structures. Then, for instance, the homometric operation RP reduces to the rotation R and the condition of the self-homometry reduces to the agreement of the vector sets in the structure in Fig. 4(*a*). Consequently, the both definitions, the self-homometry and the vector set symmetry, become the same.

We can not expect to derive any other useful and effective theorems from this wrongly formulated trivial first theorem. However, let us examine the second theorem of vector symmetry by itself. The second theorem reads:

"When a structure X is not properly self-homometric, the necessary condition for X to be vector-symmetric is that each of the points in X belongs to an orbit of such a space group K_i as with a point group isomorphic with the point group of the vector symmetry of X."

In the second theorem, it is not clear what means "X to be vector-symmetric". X is always G_V or G_V/G_I-vector symmetric by the description of S-O. That this phrase is contentless is easily seen if we recall "a man to be a mammal". If we interpret the phrase that the diffraction symmetry is different from the point group generated by an inversion and the point group of the crystal, we can proceed in our discussion. According to S-O, an orbit of vector $\boldsymbol{r}$ with respect to a group G is the set of the equivalent vectors with $\boldsymbol{r}$ with respect to G, then the orbit should be expressed by

$$Ob(\boldsymbol{r}, G)=\{g\boldsymbol{r};\ g\in G\}. \tag{39}$$

The definiton (39) of orbit agrees with that of Brown, Bülow, Neubüser, Wondratschek and Zassenhaus (1978). When the point $\boldsymbol{r}$ is at a general position and the group G is the space group of a crystal, the orbit agrees with a regular point system. Since "X is not proper self-homometric" means that X is either an ordinary structure or composite one consisting of substructures of which symmetries are called local symmetries, the second theorem can be rewritten by:

"When a structure consists of substructures, if diffraction symmetry of X is different from the point group generated by an inversion and the point group of X, the set of the position vectors of X should be expressed by

$$X=\sum_i\sum_j Ob(\boldsymbol{r}_j, K_i), \tag{40}$$

where the point group of the space group K_i is the vector-symmetry of X."

If we apply our theorem to the structures shown in Figs. 1, 2 and 3, the only structure expressed by Eq. (40) is the one in Fig. 3. The validity of this theorem is lost if only a counter-example is found. The counter-examples of this theorem can be obtained systematically by the method of Takahashi (1977). We choose a space group G of which normal subgroup G_N has different diffraction symmetry from that of G. Let us denote G by

$$G=G_N+(B, \boldsymbol{b})G_N.$$

We construct a structure X_1 of which space group is G_N and another structure X_2 which is obtained from X_1 by operating B on X_1. Then, we compose a structure X by X_1 and X_2 of which origin is displaced by $\boldsymbol{b}_t$ from that of X_1. If $\boldsymbol{b}_t=\boldsymbol{b}$, the structure X becomes ordinary one and the space group of X becomes G. If $\boldsymbol{b}_t\neq\boldsymbol{b}$, there is posibility that diffraction enhancement of symmetry occurs. For example, when G is $P4/mmm$ and G_N is $P4/m$, $(B, \boldsymbol{b})$ becomes a mirror operation. If the space group of X_1 is $P4/m$ and X_2 is the mirror image of X_1 and $\boldsymbol{b}_t=(0\ 0\ \frac{1}{4})$, the diffraction symmetry of X becomes $4/mmm$, although the space group of X is $P4$, see Appendix C.

The present author concludes that the second theorem is stated without any theoretical ground and expresses formally our expectation that the diffraction symmetries of

the structures composed of several substructures should have the rotations of the space group operations of the substructures as their elements.

6. Remarks

a) Union of sets

Union of two disjoint sets A and B, $A \cup B$, is expressed by direct sum $A+B$. Since each subsets $h_i^{-1}K_0h_j$ in M are disjoint, M can be expressed by Eq. (8) instead of Eq. (1) of S-O.

b) Equivalent operation with h_i

An operation belonging to hull h_i is equivalent with $(E, \boldsymbol{n})h_i$,

$$(E, \boldsymbol{n})h_i = (B_i^{-1}, -B_i^{-1}\boldsymbol{b}_i + \boldsymbol{n})$$

where $(E, \boldsymbol{n})$ is an element of the translation group T.

c) Partial operations

A very important term used by S-O is "partial operation", which is not discussed in the preceding sections. According to S-O, "It operates only on a subspace A of a crystal space to bring it to superposition upon another B and is accordingly not a symmetry operation." The partial operations can be defined if we can define the subspaces on which the operations operate. On the contrary to S-O, the symmetry operations between substructures, $(B_i, \boldsymbol{b}_i)$, which shoud belong to the hull of a groupoid, operate over all the crystal space for the structures consisting of substructures. The operations are not partial operations by the definition of S-O.

Another kind of partial operations was introduced by S-O. According to S-O, a structure A can be brought onto another homometric structure B by the set of the partial

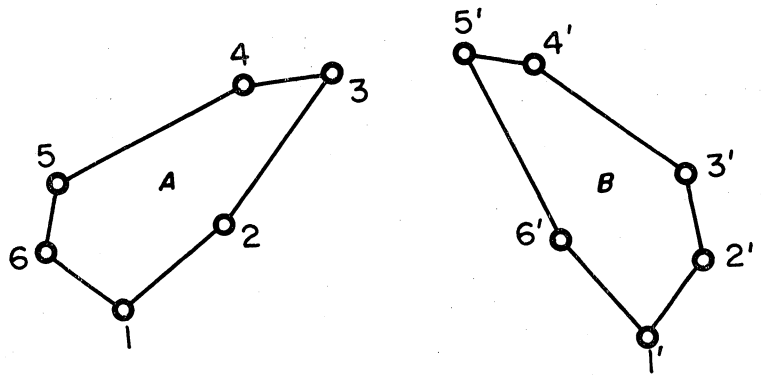

Fig. 5. Fig. 4 (*b*) of S-O. The points are numbered by the present author.

operations which bring the inter-point vectors in A onto those in B. Figure 5 is an enlarged copy of Fig. 4(b). The points in A and B are numbered. In order to bring an inter-point vector $\boldsymbol{r}_i-\boldsymbol{r}_j$ in A onto $\boldsymbol{r}_{s'}-\boldsymbol{r}_{t'}$ in B, we must rotate $\boldsymbol{r}_i-\boldsymbol{r}_j$ by $\pi/2$ and translate parallel the vector so as to make agree $\boldsymbol{r}_j$ with $\boldsymbol{r}_{t'}$. Hence, a partial operation S_k operates on the element of V and that of X, that is,

$$S_k(\boldsymbol{r}_i-\boldsymbol{r}_j, \boldsymbol{r}_j)=(\boldsymbol{r}_{s'}-\boldsymbol{r}_{t'}, \boldsymbol{r}_{t'}).$$

For example, the five partial operations operating on the inter-point vectors directed from the 1st point to the 2nd, 3rd, 4th, 5th and 6th points in A can be expressed by

$$\begin{aligned}
S_1(\boldsymbol{r}_2-\boldsymbol{r}_1, \boldsymbol{r}_1)&=(\boldsymbol{r}_6'-\boldsymbol{r}_1', \boldsymbol{r}_1'),\\
S_2(\boldsymbol{r}_3-\boldsymbol{r}_1, \boldsymbol{r}_1)&=(\boldsymbol{r}_5'-\boldsymbol{r}_2', \boldsymbol{r}_2'),\\
S_3(\boldsymbol{r}_4-\boldsymbol{r}_1, \boldsymbol{r}_1)&=(\boldsymbol{r}_5'-\boldsymbol{r}_3', \boldsymbol{r}_3'),\\
S_4(\boldsymbol{r}_5-\boldsymbol{r}_1, \boldsymbol{r}_1)&=(\boldsymbol{r}_6'-\boldsymbol{r}_3', \boldsymbol{r}_3'),\\
S_5(\boldsymbol{r}_6-\boldsymbol{r}_1, \boldsymbol{r}_1)&=(\boldsymbol{r}_2'-\boldsymbol{r}_1', \boldsymbol{r}_1').
\end{aligned}$$

When A has n points, the number of the inter-point vectors from the ith point to the other point in A is $n-1$. The $n-1$ vectors are brought by $n-1$ partial operations to $n-1$ vectors in B. The $n-1$ vectors in B do not have a common point which corresponds to the ith point in A. If there is a common point, the operations become an oridinary rotation. The subspaces in A on which the $n-1$ partial operations operate do not contain the ith point. Since there is no point corresponding to the ith point in B, the subspaces in A which are brought to those of B by all the partial operations do not contain the n points of A, that is, there are no partions which bring A to B.

Appendix A

According to Burckhardt (1966), an element $(A_i, \boldsymbol{a}_i)$ of a space group G can be represented by another equivalent form $(B_i, \boldsymbol{b}_i)$ satisfying

$$(U, \boldsymbol{s})^{-1}(A_i, \boldsymbol{a}_i)(U, \boldsymbol{s})\equiv(B_i, \boldsymbol{b}_i) \pmod{T}. \tag{A-1}$$

In the theory of Burckhardt, the bases of representations of space groups are primitive reduced, and the translation groups for any space groups are represented by

$$T=\{(E, \boldsymbol{n});\ \text{the elements of } \boldsymbol{n} \text{ are any integers}\}. \tag{A-2}$$

It must be noticed that there are different but equivalent representations for a space

group eventhough the bases of the representation are the same. In general, two equivalent representations G_1 and G_2 for a space group G,

$$G_1 = T_1(E, 0) + T_1(A_2, \boldsymbol{a}_2) + \cdots\cdots \tag{A-3}$$

and

$$G_2 = T_2(E, 0) + T_2(B_2, \boldsymbol{b}_2) + \cdots\cdots \tag{A-4}$$

must satisfy

$$(U, \boldsymbol{s})^{-1} T_1(U, \boldsymbol{s}) = T_2, \tag{A-5}$$

in addition to (A−1), where

$$(U, \boldsymbol{s})^{-1} T_1(U, \boldsymbol{s}) = \{(U, \boldsymbol{s})^{-1} t(U, \boldsymbol{s});\ t \in T_1\}. \tag{A-6}$$

If a space group G has a normal subgroup H,

$$G = H + gH, \tag{A-7}$$

points in a structure X satisfying

$$\boldsymbol{r} = \boldsymbol{gr} \tag{A-8}$$

form a subset X_s of X, the subset including X_s and its equivalent subsets with respect to H is transformed onto itself by the elements of G. We can form two sets $X_H(\boldsymbol{r})$ and $X_{gH}(\boldsymbol{r})$ from a point $\boldsymbol{r}$ belonging to X_s,

$$X_H(\boldsymbol{r}) = \{\boldsymbol{hr};\ h \in H\} \tag{A-9}$$

and

$$X_{gH}(\boldsymbol{r}) = \{\boldsymbol{ghr};\ h \in H\}. \tag{A-10}$$

Since $g^2 = e$ and $H = g^{-1}Hg$, the set $X_{gH}(\boldsymbol{r})$ agrees with $X_H(\boldsymbol{r})$,

$$\begin{aligned} X_{gH}(\boldsymbol{r}) &= \{\boldsymbol{ghr};\ h \in H\} \\ &= \{\boldsymbol{ghgr};\ h \in H\} \\ &= \{\boldsymbol{hr};\ h \in H\} \\ &= X_H(\boldsymbol{r}). \end{aligned} \tag{A-11}$$

Hence,

$$X(\boldsymbol{r})=X_H(\boldsymbol{r})\cup X_{gH}(\boldsymbol{r})$$
$$=X_H(\boldsymbol{r}). \tag{A-12}$$

When two inequivalent space groups G_1 and G_2, which are generated from the same point group, have a common normal subgroup H,

$$G_1=H+g_1H \quad \text{and} \quad G_2=H+g_2H, \tag{A-13}$$

if

$$g_1\boldsymbol{r}_1=\boldsymbol{r}_1 \quad \text{and} \quad g_2\boldsymbol{r}_2=\boldsymbol{r}_2, \tag{A-14}$$

the sets of the position vectors $X_1(\boldsymbol{r}_1)$ and $X_2(\boldsymbol{r}_2)$,

$$X_1(\boldsymbol{r}_1)=\{g\boldsymbol{r}_1;\ g\in G_1\} \quad \text{and} \quad X_2(\boldsymbol{r}_2)=\{g\boldsymbol{r}_2;\ g\in G_2\}, \tag{A-15}$$

are invariant by the operations belonging to H, but $X_1(\boldsymbol{r}_1)$ and $X_2(\boldsymbol{r}_2)$ are changed by g_2 and g_1, respectively. There is no transformation changing $X_1(\boldsymbol{r}_1)$ to $X_2(\boldsymbol{r}_2)$.

Appendix B

The set X of the position vectors of a structure A can be expressed by the sum of delta functions,

$$D_A=\sum_i^{N_A}\delta(\boldsymbol{r}-\boldsymbol{r}_i{}^A). \tag{B-1}$$

The convolution of D_A and D_B results

$$D_{A*B}=\sum_i^{N_A}\sum_j^{N_B}\delta(\boldsymbol{r}-\boldsymbol{r}_i{}^A-\boldsymbol{r}_j{}^B). \tag{B-2}$$

Hence, the set X_{A*B} of the position vectors of the structure $A*B$ becomes

$$X_{A*B}=\{\boldsymbol{r}_i{}^A+\boldsymbol{r}_j{}^B;\ i\leq N_A, j\leq N_B\}, \tag{B-3}$$

and V_{A*B} is

$$V_{A*B}=\{\boldsymbol{r}_i{}^A+\boldsymbol{r}_j{}^B-\boldsymbol{r}_k{}^A-\boldsymbol{r}_m{}^B;\ i,k\leq N_A, j,m\leq N_B\}. \tag{B-4}$$

We have the following very useful relations for homometry. "If

$$A\overset{h}{=}C \quad \text{and} \quad B\overset{h}{=}D, \tag{B-5}$$

then

$$A*B\overset{h}{=}C*B\overset{h}{=}A*D\overset{h}{=}C*D.\text{"} \tag{B-6}$$

The proof of the first homometry is as follows. Since $A\overset{h}{=}C$, there are always vectors satisfying

$$\boldsymbol{r}_i{}^A-\boldsymbol{r}_k{}^A=\boldsymbol{r}_{i'}{}^C-\boldsymbol{r}_{k'}{}^C \tag{B-7}$$

in V_A and V_C, hence

$$\begin{aligned} V_{A*B}&=\{\boldsymbol{r}_i{}^A+\boldsymbol{r}_j{}^B-\boldsymbol{r}_k{}^A-\boldsymbol{r}_m{}^B;\ i,k\leq N_A, j,m\leq N_B\}\\ &=\{\boldsymbol{r}_{i'}{}^C+\boldsymbol{r}_j{}^B-\boldsymbol{r}_{k'}{}^C-\boldsymbol{r}_{m'}{}^B;\ i',k'\leq N_C, j,m\leq N_B\}\\ &=V_{C*B}. \end{aligned} \tag{B-8}$$

The other homometries in (B-6) can be proved similarly.

Appendix C

When a set X of position vectors is given by direct sum of the subsets X_i,

$$X=\sum_i X_i, \tag{C-1}$$

if a function $f(X)$ of the elements of X is additive with respect to the subsets,

$$f(X)=\sum_i f(X_i), \tag{C-2}$$

the symmetry G of $f(X)$ satisfies

$$G\supseteq\bigcap_i G_i, \tag{C-3}$$

where G_i is the symmetry of $f(X_i)$.

Structure factor $F(\boldsymbol{h},X)$ is additive,

$$F(\boldsymbol{h},X)=\sum_i F(\boldsymbol{h},X_i), \tag{C-4}$$

the symmetry of the structure factor satisfies (C-3). Vector set $V(X)$ is not additive,

$$V(X)\neq\sum_i V(X_i), \tag{C-5}$$

the symmetry of $V(X)$ does not satisfy (C-3). Although the absolute value of the structure factor $F(\boldsymbol{h},X)$ is not additive in general,

$$|F(\boldsymbol{h},X)|\neq\sum_i|F(\boldsymbol{h},X_i)|, \tag{C-6}$$

if the arguments of $F(\boldsymbol{h}, X_i)$ are equal to each other, the absolute value of the structure factor $F(\boldsymbol{h}, X)$ becomes additive, the symmetry of the absolute value satisfies (C-3). This case is *type* 1 of Iwasaki (1972), see Takahashi (1977). If the number of the subsets in X is two and

$$F(\boldsymbol{h}, X_1)\cdot F(\boldsymbol{h}, X_2)=0 \qquad \text{for } \boldsymbol{h}\neq\boldsymbol{h}_0, \tag{C-7}$$

where $\boldsymbol{h}_0$ is the origin of the reciprocal lattice, the reciprocal lattice space can be divided into two subspaces H_1 and H_2 satisfying

$$F(\boldsymbol{h}, X_1)=0 \qquad \text{for } \boldsymbol{h}\in H_1 \text{ and } \boldsymbol{h}\neq\boldsymbol{h}_0, \tag{C-8}$$

$$F(\boldsymbol{h}, X_2)=0 \qquad \text{for } \boldsymbol{h}\in H_2 \text{ and } \boldsymbol{h}\neq\boldsymbol{h}_0, \tag{C-9}$$

and

$$H_1\cap H_2=\{\boldsymbol{h}_0\}. \tag{C-10}$$

If diffraction symmetry of $F(\boldsymbol{h}, X_1)$ and $F(\boldsymbol{h}, X_2)$ are the same, the diffraction enhancement of symmetry of *type* 3 of Iwasaki (1972) occurs.

Let us assume that a structure consists of two substructures of which space groups are $P4/m$. The symmetry between substructures $(\boldsymbol{B}, \boldsymbol{b}_t)$ is assumed by

$$\boldsymbol{B}=\begin{bmatrix} 1 & 0 & 0 \\ 0 & \bar{1} & 0 \\ 0 & 0 & \bar{1} \end{bmatrix} \text{ and } \boldsymbol{b}_t=\begin{bmatrix} 0 \\ 0 \\ 1/4 \end{bmatrix}$$

The set of the position vectors of atoms in the unit cell is direct sum of the sets of the position vectors in each of substructures,

$$X=X_1+X_2,$$

where

$$X_1=\sum_i\{g\boldsymbol{r}_i;\ g\in P4/m\}$$

and

$$\begin{aligned} X_2&=\sum_i\{mg\boldsymbol{r}_i+\boldsymbol{b}_t;\ g\in P4/m\} \\ &=\sum_i(\boldsymbol{b}_t+\{mg\boldsymbol{r}_i;\ g\in P4/m\}) \\ &=(\boldsymbol{b}_t+mX_1) \end{aligned}$$

The trigometric part of the structure factor of an atom at $\boldsymbol{r}$ and its equivalent atoms with respect to $P4/m$ is given by

$$f(\boldsymbol{h}, \boldsymbol{r}) = 4\cos(2\pi lz)(\cos(2\pi(hx+ky)) + \cos(2\pi(\bar{h}y+kx))).$$

The structure factor $F(\boldsymbol{h}, X)$ of the structure X is obtained by summing $f(\boldsymbol{h}, \boldsymbol{r}_i)$ multiplied by scattering factor f_i over all the elements in X_1,

$$F(\boldsymbol{h}, X) = F(\boldsymbol{h}, X_1) + \exp(\tfrac{1}{2}\pi il)F(\boldsymbol{h}, mX_1)$$

where

$$F(\boldsymbol{h}, X_1) = \sum_i f_i f(\boldsymbol{h}, \boldsymbol{r}_i)$$

and

$$F(\boldsymbol{h}, mX_1) = \sum_i f_i f(\boldsymbol{h}, m\boldsymbol{r}_i).$$

If m is operated on $F(\boldsymbol{h}, X)$, $F(\boldsymbol{h}, X)$ is transformed to

$$\begin{aligned} mF(\boldsymbol{h}, X) &= F(\boldsymbol{h}, mX_1) + \exp(-\tfrac{1}{2}\pi il)F(\boldsymbol{h}, X_1) \\ &= \exp(-\tfrac{1}{2}\pi il)(F(\boldsymbol{h}, X_1) + \exp(\tfrac{1}{2}\pi il)F(\boldsymbol{h}, mX_1)). \end{aligned}$$

The absolute value of $mF(\boldsymbol{h}, X)$ is equal to $F(\boldsymbol{h}, X)$. The operation m becomes an element of the diffraction symmetry of the structure. The diffraction symmetry becomes $4/mmm$.

Postscript

This paper was submitted to Acta Crystallographica and rejected finally by the editor S. C. Abrahams. The editor's letter and his referee's comment are shown in Fig. 5. The referee's comment is only repetition of Sadanaga and Ohsumi. The author wonders if the editor, co-editors and referees of Acta Crystallographica believe truely that space-groupoid theory of Sadanaga and Ohsumi can be compatible with space group theory. If so, they lack incredibly the knowledge of set theory which is a foundation of group theory. If not, they lack sincerity for science. This postscript is for the evidence of the author's struggle for nearly two decades against space-groupoid theory in the future.

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March 3, 1983

AIRMAIL

Dr. H. Takahashi
Faculty of Education
Kagoshima University
Kagoshima
JAPAN

Dear Dr. Takahashi:

The referee for your revised manuscript, number SA043, has completed his report which is enclosed herewith. The referee does not recommend publication in Acta Crystallographica.

In view of this recommendation, which confirms that made by the five previous referees, it is regretfully concluded that this paper is unacceptable for Acta Crystallographica. The basic misunderstanding identified in the paper leaves no doubt that further revisions will continue to be unacceptable, hence it should not be resubmitted.

The original copy of your manuscript is returned together with the report. Your interest in Acta Cystallographica is indeed appreciated.

Sincerely yours,

S. C. Abrahams

Re. No.SA043, "Examination of Space-Groupoid Theory, I. Theory of Sadanaga and Ohsumi" by Hidewo Takahashi

In general, a trigonal crystal gives a trigonal diffraction pattern. In particular, however, the trigonal 10H polytype of SiC produces a hexagonal diffraction pattern (Ramsdell, L. S. and Kohn, J. A. (1951) Acta Cryst. 4, 111-113). Hence, we know that the diffraction symmetry of a crystal can be higher than its Laue symmetry. Then, with what kind of symmetric feature of a crystal is its diffraction symmetry is related ? This is the question which prompted Sadanaga and Ohsumi to their study of vector symmetry.

The referee thinks that we had better deal with finite patterns because these offer a clearer view of Sadanaga and Ohsumi's conclusion than that deduced from infinite patterns like crystal structures, and let us call our finite patterns 'molecules'. The diffraction symmetry of a molecule is the same as the symmetry of the vector set of the molecule. Sadanaga and Ohsumi treated the symmetry G_V of the vector set of a structure X with their concept of self-homometry of X and related G_V with symmetric features of X. In terms of molecule X, we can reiterate Sadanaga and Ohsumi's result as follows, where G_X is the point group of X and G_I an inversion group;

(1) If there is in X a point which belongs to neither an orbit of G_V nor an orbit of G_V/G_I, G_V is due to the 'proper self-homometry' of X (Fig.4 in Sadanaga and Ohsumi's paper).
(2) If each point in X belongs to an orbit of G_V or G_V/G_I, two cases are possible as follows:
  (2a) If G_X is siomorphic with G_V or G_V/G_I, X is an ordinary point-group molecule;
  (2b) If G_X is not isomorphic with G_V or G_V/G_I, X is a groupoid molecule consisting of sub-molecules for

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which G_V or G_V/G_I is a common point group, where G_V and G_V/G_I in (2) correspond respectively to G_V and G_V/G_I in (2a) and (2b).

If Figs. 6, 7 and 8 in Sadanaga and Ohsumi's paper are looked upon, not as the unit-cell content of a crystal structure, but as a finite pattern - a molecule, these come under (2b) in the above classification.

Next, let us take Fig.7 and regard it as a molecule consisting of sixteen equal atoms. As simple geometric consideration reveals, the vector set of this molecule is tetragonal. Though the molecule as a whole is not tetragonal, each atom belongs to a tetragonal orbit, and its point group, 4, constitutes the kernel of this groupoid. Every element of the hull involves a similarity transformation. In order to visualize this point, let us look at Fig.2 in Takahashi's manuscript. Turn the square denoted as (1234) around the point marked 3 so as for 2 to be in line with 3 and 2' and for 4 in line with 3 and 4'. Next, dilate the square in this new position, by keeping its square shape and with point 3 fixed, until 2 and 4 coincide 2' and 4' respectively, (1234) will now be transformed into (1'2'34'). In this way, we shall recognize that an element of the hull is a combination of either a rotation and a dilatation or a rotation, a translation and a dilatation. However, we need not stick to these operations; we can simply define this element of the hull as one of one-to-one mappings: 1 → 1', 2 → 2', 3 → 3, 4 → 4'; 1 → 2' 2 → 3, 3 → 4', 4 → 1'; and so on.

Introduction of non-crystallographic operations as elements of the hull of a groupoid as done by Sadanaga and Ohsumi is by no means a violation of the theory of space groups, the space group being conserved in their space groupoid in the form of its kernel. In general, as long as all the substructures constructing a structure bear the same symmetry, an operation

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relating arbitrarily chosen two substructures with each other can be defined quite freely, even as a one-to-one mapping of one onto the other. No one is entitled to suppress this freedom in the name of crystallography.

In conclusion, because the present manuscript is based upon Takahashi's misunderstanding of Sadanaga and Ohsumi's paper, the referee regrets to say that he is not in favor of its publication in Acta Crystallographica.

Fig. 6. The letter of S.C. Abrahams, Editor of Acta Crystallographica, and the referee's comment.

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