mitted modes N_p, are listed. The permitted modes are those with positive μ or positive y^r. Clearly, the number of permitted modes satisfies the relation, $N_p = 2(N - N_{\rm Bragg})$.

III. Discussion and conclusion

With the above considerations, it has been shown that at the exact N-beam diffraction position y^r and μ always have the same sign. As mentioned above, the absorption coefficient of a permitted mode must be positive. The permitted mode should always have positive y^r associated with it. For both σ- and π-polarized wavefields, the number of modes having negative absorption coefficients, according to (13) and Table 1, is equal to $2N_{\rm Bragg}$. The number of permitted modes is then the number of the rest of the modes, *i.e.* $2N - 2N_{\rm Bragg}$. In other words, it is twice the number of transmitted beams, including the incident one. This is exactly consistent with the characteristics of two-beam cases discussed above. Apparently, this relation also holds for N-beam Borrmann diffraction, in which no Bragg reflections are involved. The number of permitted modes equals the number of total possible modes, $2N$.

Although this relation is quite general, it is not applicable to those cases which involve extremely asymmetric reflections. For such cases, higher-order terms of (Δk) need to be considered. This leads to more permitted modes since the equation of dispersion has the form of a high-order polynomial. Besides, extra modes may be introduced by some related physical phenomenon, such as the specular reflection of X-rays from the crystal surface where the glancing angle of the incident beam is less than 1 or 2° (Kishino & Kohra, 1971).

Nevertheless, without extremely asymmetric reflection in N-beam dynamical diffraction, the relation $N_p = 2(N - N_{\rm Bragg})$ holds as a general rule for determining the number of permitted modes of wave propagation. As stated before, the diffracted intensities can be calculated by solving the equations obtaining from the boundary conditions for these N_p wavefields. Based on this, the interpretation of *Aufhellung* (Wagner, 1923; also quoted by Mayer, 1928) and *Umwegangregung* (Renninger, 1937) effects in terms of the dynamical theory of diffraction is possible.

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Derivation of Possible Framework Structures Formed from Parallel Four- and Eight-Membered Rings

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Abstract

The number of possible combinations of parallel four-membered rings, of the same kind, forming an eight-membered ring is systematically derived by a different method from that of Smith & Rinaldi [*Mineral. Mag.* (1962). **33**, 202–211]. 17 different configurations (including six enantiomorphic) in the *UUDD* ring (*U* and *D* represent upward- and downward-pointing tetrahedra respectively), four different ones (two enantiomorphic) in the *UDUD* ring, and sixteen different ones (seven enantiomorphic) in the *UUDD* ring are shown

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with their new pattern representations and symbol notations.

Introduction

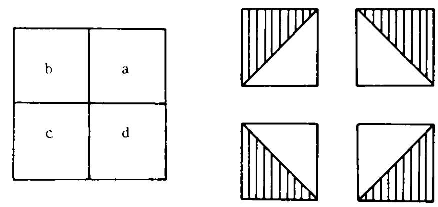
A simple convenient symbolism was developed by Smith & Rinaldi (1962) in order to classify and describe framework structures which are formed from parallel four- and eight-membered rings of TO_4 (T = Al, Si) tetrahedra. According to them, possible four-membered rings can be represented in terms of the codes *UUDD*, *UDUD*, *UUUD*, and *UUUU*, where the symbols *U* and *D* denote an upward and a downward pointing tetrahedron respectively. Various eight-membered rings can be formed by combining these four-membered rings. Imposing a restriction on repeat distances in the plane (less than 15 Å), Smith & Rinaldi (1962) showed that there are 17 possible different configuration types for the arrangement of the *UUDD* ring, four types for the *UDUD* ring, seven types for the *UUUD* ring, and one type for the *UUUU* ring. However, there are no detailed explanations of the numbers of possible configurations, or of the relation between the symbol notation and the configuration. These problems are important as a first step towards consideration of more complex framework structures. This paper presents a different systematic derivation of the possible combinations, and a new notation system for the configurations.

In the following treatment, various restrictions such as the repeating distances, or the parallelism of four- and eight-membered rings are the same as in Smith & Rinaldi (1962), and the trivial case of the *UUUU* ring is not discussed.

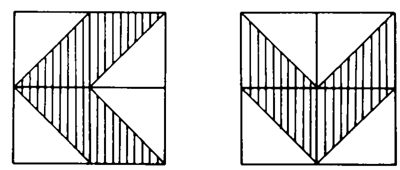
Configurations based on the *UUDD* ring

Fig. 1(*a*) is a structure model of harmotome ($BaAl_2Si_6O_{16}.6H_2O$), and Fig. 1(*b*) the symbolized model of Smith & Rinaldi (1962). Now if we represent one *UUDD* ring by one square tile consisting of black and white triangles, in which a black triangle denotes the *DD* and a white one the *UU*, then the harmotome configurations can be shown as a tile arrangement pattern, as shown in Fig. 1(*c*). It can be also considered that this pattern is formed by putting four square tiles with different orientations into the four distinct boxes. Then the enumeration of possible combinations of the four-membered *UUDD* ring becomes equivalent to counting the number of different arrangement patterns of the tiles in the four boxes.

Let the four boxes on a 2 × 2 board be denoted as *a*, *b*, *c* and *d*. Then each box can accept independently four differently oriented tiles as shown in Fig. 2(*a*).



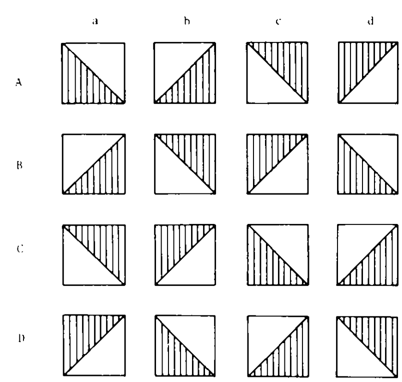
(*a*)



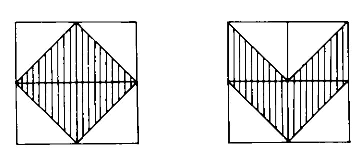
(1) (2)

(*b*)

Fig. 2. (*a*) Four boxes *abcd* (left) and four different tile orientations (right). (*b*) Two rotationally equivalent patterns.

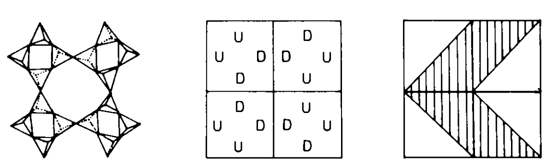


(*a*)



(*b*)

Fig. 3. (*a*) Four different tile orientations (*A*,*B*,*C*,*D*) in four distinct boxes (*a*,*b*,*c*,*d*) in the *UUDD* ring. (*b*) Two examples of pattern-notation symbols.



(*a*) (*b*) (*c*)

Fig. 1. Three different representations of the harmotome structure ($BaAl_2Si_6O_{16}.6H_2O$). (*a*) Original harmotome structure showing linkage between (Si, Al)O_4 tetrahedra (Sadanaga, Marumo & Takéuchi, 1961). (*b*) *UUDD* symbol representation by Smith & Rinaldi (1962). (*c*) Pattern representation using black and white tiles.

Therefore the total number of possible arrangement patterns is $4 \times 4 \times 4 \times 4 = 256$. However, there are many rotationally equivalent patterns among them. Two patterns are rotationally equivalent if one can be transformed into the other by a rotation around the center of the board. One example is shown in Fig. 2(*b*), in which pattern (1) is transformed into pattern (2) by a 90° anticlockwise rotation, and pattern (2) into pattern (1) by a similar clockwise rotation.

We first count the total number of rotationally non-equivalent patterns using combinatorial mathematics. As stated above, a tile can take four orientations, which we call A, B, C and D in box a. The orientations B, C, and D can be obtained by transforming orientation A by 90, 180 and 270° anticlockwise rotations respectively, which are shown in the first column a in Fig. 3(*a*). Now the tile in the box a can be transformed into the box b by a 90° anticlockwise rotation around the center of the board. In this operation, the orientations A, B, C and D in box a can be transformed into the new orientations shown in column b, which we call the orientations A, B, C and D in box b. Performing successive rotations, new orientations A, B, C and D in boxes c and d can be obtained. Using these orientation notations, any tile arrangement pattern can be represented simply by its sequence of orientation symbols in the order of boxes a, b, c and d. Two examples are shown in Fig. 3(*b*). One more advantage of this notation system is that all equivalent patterns can be expressed in terms of a cyclic permutation of the starting orientation symbol. Thus a pattern denoted by the symbol $BDAA$ is equivalent to those denoted by $DAAB$, $AABD$ and $ABDA$. Now we will count all the non-equivalent sequences. Let $D = \{a, b, c, d\}$ be a set of four boxes on a board and $R = \{A, B, C, D\}$ a set of four orientations of tiles. We can specify a cyclic group C_4 as a permutation group G acting on set D:

$$G = \left\{ \begin{pmatrix} abcd \\ abcd \end{pmatrix}, \begin{pmatrix} abcd \\ bcda \end{pmatrix}, \begin{pmatrix} abcd \\ cdab \end{pmatrix}, \begin{pmatrix} abcd \\ dabc \end{pmatrix} \right\}.$$

Then the cyclic index of cyclic group C_4 is

$$Z(C_4) = \tfrac{1}{4}(x_1^4 + x_2^2 + 2x_4),$$

and the figure counting series

$$e(u, v, w, z) = u + v + w + z,$$

(Berge, 1971). Substituting the latter into the former equation, we can obtain

$$Z(C_4, u + v + w + z) = \tfrac{1}{4}[(u + v + w + z)^4 + (u^2 + v^2 + w^2 + z^2)^2 + 2(u^4 + v^4 + w^4 + z^4)].$$

The coefficient of $u^l v^m w^n z^p$ in the polynomial expansion is the number of different sequences with four symbols, l A's, m B's, n C's and p D's. The sum of each coefficient gives us the total number of non-equivalent symbol sequences. The number of symbol sequences can also be counted by using $3 + u$ as the figure counting series instead of $u + v + w + z$, where the weight 1 is given for symbol A and the weights 0 for all the others. Then in

$$Z(C_4, 3 + u) = \tfrac{1}{4}[(3 + u)^4 + (3 + u^2)^2 + 2(3 + u)^4]$$
$$= u^4 + 3u^3 + 15u^2 + 27u + 24,$$

the coefficient of u^l shows the number of symbol sequences with l A's. Thus we know that there is 1 sequence with 4 A's, 3 sequences with 3 A's, 15 sequences with 2 A's, 27 sequences with 1 A, and 24 sequences without A, the total number being 70.

The derived sequences are shown in Table 1. It is very easy to draw out the corresponding pattern from the given symbol sequence. The 70 patterns corresponding to these 70 sequence symbols are basic unit patterns which extend to form infinite repeating patterns on the plane. It is true that they are not rotationally equivalent, but they are not necessarily independent of each other in the translational relation. The reason for

Table 1. 70 *rotationally non-equivalent configuration symbols in the UUDD ring*

The numerical values in the right-hand column are numbers of members involved in the subgroup, corresponding to the coefficients of u in the polynomial expansion $Z(C_4, 3 + u)$.

AAAA						(1)
AAAB						
AAAC						(3)
AAAD						
AABB	*ABAB*					
AACC	*ACAC*					
AADD	*ADAD*					(15)
AABC	*AACB*	*ACAB*				
AABD	*AADB*	*ADAB*				
AACD	*AADC*	*ADAC*				
ABBB						
ACCC						
ADDD						
ABBC	*ABCB*	*ACBB*				
ABBD	*ABDB*	*ADBB*				
ACCB	*ACBC*	*ABCC*				
ACCD	*ACDC*	*ADCC*				(27)
ADDB	*ADBD*	*ABDD*				
ADDC	*ADCD*	*ACDD*				
ABCD	*ACBD*	*ADCB*	*ABDC*	*ACDB*	*ADBC*	
BBBB						
CCCC						
DDDD						
BBBC						
BBBD						
CCCB						
CCCD						
DDDB						
DDDC						
BBCC	*BCBC*					
BBDD	*BDBD*					
CCDD	*CDCD*					
BCCD	*BCDC*	*BDCC*				(24)
BCDD	*BDCD*	*CBDD*				
BBCD	*BBDC*	*BDBC*				

this is as follows: Fig. 4 shows a pattern constructed from four unit patterns of *AAAA*, and we can see that the pattern contains not only one pattern of *AAAA*, but also two other non-equivalent patterns denoted by *DBDB*(*BDBD*) and *CCCC*. The pattern *DBDB*(*BDBD*) is obtained by shifting the rotation center by $\mathbf{t}_2/2$ (or $\mathbf{t}_1/2$), and the pattern *CCCC* by shifting by $(\mathbf{t}_1 + \mathbf{t}_2)/2$, where $\mathbf{t}_1$ and $\mathbf{t}_2$ are repeating vectors along the x and y directions. We can say that they are translationally related. The derivation of these translationally related patterns can be performed by drawing out all adjacent patterns, but the procedure is very tedious. One convenient method is presented in the following. Let X be a set of four boxes a, b, c, d, and R be three cyclic permutation operations r^1, r^2, r^3, *i.e.*,

$$X = \{a, b, c, d\}, \quad R = \{r^1, r^2, r^3\},$$

where

$$r^1 = \begin{pmatrix} ABCD \\ DABC \end{pmatrix}, \quad r^2 = \begin{pmatrix} ABCD \\ CDAB \end{pmatrix}, \quad r^3 = \begin{pmatrix} ABCD \\ BCDA \end{pmatrix}.$$

Then the translation of the rotation center by $\mathbf{t}_1/2$ causes a change of orientation symbols, which can be expressed by mapping X into R (Berge, 1971),

$$\varphi_{\mathbf{t}_1/2} = \begin{pmatrix} a & b & c & d \\ r^1 & r^3 & r^1 & r^3 \end{pmatrix}.$$

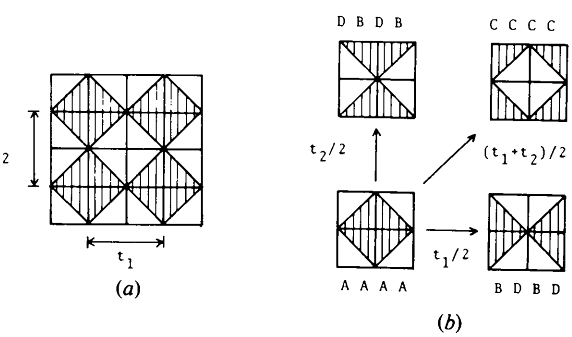


Fig. 4. (*a*) A composite pattern constructed from four unit patterns of *AAAA*. (*b*) Four translationally related patterns which are produced by shifting an original rotation center by $\mathbf{t}_1/2$, $\mathbf{t}_2/2$ and $(\mathbf{t}_1 + \mathbf{t}_2)/2$ respectively.

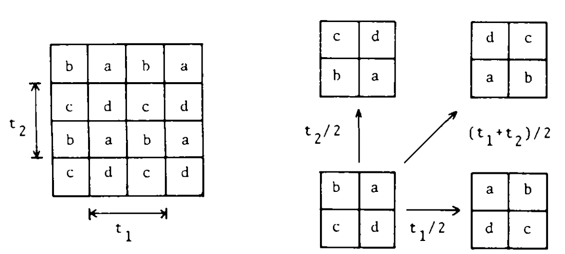


Fig. 5. Box sequence change resulting from shifting of the rotation center.

Similarly, for the translations $\mathbf{t}_2/2$ and $(\mathbf{t}_1 + \mathbf{t}_2)/2$ the changes can be expressed as

$$\varphi_{\mathbf{t}_2/2} = \begin{pmatrix} a & b & c & d \\ r^3 & r^1 & r^3 & r^1 \end{pmatrix}, \quad \varphi_{(\mathbf{t}_1+\mathbf{t}_2)/2} = \begin{pmatrix} a & b & c & d \\ r^2 & r^2 & r^2 & r^2 \end{pmatrix}.$$

The box sequence *abcd* must be also changed into the sequences *badc*, *dcba*, and *cdab* for the translations $\mathbf{t}_1/2$, $\mathbf{t}_2/2$ and $(\mathbf{t}_1 + \mathbf{t}_2)/2$ respectively (Fig. 5). All these relations can be shown in Table 2(*a*), from which we can easily derive the translationally related sequences.

For example, starting with an original sequence *ABAD*, the procedure for obtaining the $\mathbf{t}_1/2$ translationally related sequence is as follows:

(1) Set the original sequence symbol in the order of a box sequence *abcd*

$$\begin{pmatrix} a & b & c & d \\ A & B & A & D \end{pmatrix}.$$

(2) In Table 2(*a*), select symbol D at the intersection of column a with row A, symbol C at column b with row B, symbol D at column c with row A, symbol A on column d with row D, and replace the original sequence with

$$\begin{pmatrix} a & b & c & d \\ D & C & D & A \end{pmatrix}.$$

(3) Replace the box sequence symbol *abcd* with the corresponding numbers in the bottom row

$$\begin{pmatrix} 2 & 1 & 4 & 3 \\ D & C & D & A \end{pmatrix}.$$

(4) Rearrange the sequence symbols in increasing order of the numbers

$$\begin{pmatrix} 1 & 2 & 3 & 4 \\ C & D & A & B \end{pmatrix}.$$

Table 2. *Derivation tables for translationally related and enantiomorphic symbols in the UUDD ring*

(*a*) Translationally related

	$\mathbf{t}_1/2$	$\mathbf{t}_2/2$	$(\mathbf{t}_1 + \mathbf{t}_2)/2$
	a b c d	*a b c d*	*a b c d*
A	*D B D B*	*B D B D*	*C C C C*
B	*A C A C*	*C A C A*	*D D D D*
C	*B D B D*	*D B D B*	*A A A A*
D	*C A C A*	*A C A C*	*B B B B*
	2 1 4 3	4 3 2 1	3 4 1 2

(*b*) Enantiomorphic

	a b c d
A	*A A A A*
B	*D D D D*
C	*C C C C*
D	*B B B B*
	2 1 4 3

The sequence *CDAB* is a desirable one. Two other related sequences *CBAB* and *CBCD* are similarly obtained from the same table for $\mathbf{t}_2/2$ and $(\mathbf{t}_1 + \mathbf{t}_2)/2$ respectively. The use of an electronic computer makes the derivation more easy. Thus it can be found that the 70 rotationally non-equivalent patterns are reduced to 23 translationally non-related ones, all of which are shown in Table 3. Among them, however, there are still some enantiomorphic pairs, *i.e.* left- and right-handed. They can be recognized by visual inspection, or by the following simple procedure. Let r be a cyclic permutation operation

$$r = \begin{pmatrix} A & B & C & D \\ A & D & C & B \end{pmatrix},$$

then the change of the orientation symbols by an enantiomorphic operation, in this case the mirror plane being set vertically through the center of the board, can be expressed as

$$\varphi_{\mathrm{E}} = \begin{pmatrix} a & b & c & d \\ r & r & r & r \end{pmatrix},$$

and the box sequence *abcd* is changed into the sequence *badc*. These relations are shown in Table 2(*b*), from which six pairs of enantiomorphic patterns can be derived:

AAAB and *AADA*, *AABB* and *AADD*, *ABAB* and *DADA*, *AABC* and *AACD*, *AACB* and *AADC*, *ACAD* and *CABA*.

Thus we have 17(=23 − 6) independent patterns, which are completely consistent with those of Smith & Rinaldi (1962), except for those which are enantiomorphic. All the patterns obtained are shown with their new notation symbols in Fig. 6.

Configurations based on the *UDUD* ring

In the *UDUD* ring the upward- and the downward-pointing tetrahedra alternate to form four-membered rings, and therefore there are only two kinds of tile orientations in one box as shown in Fig. 7(*a*). The cycle index is

$$Z(C_4) = \tfrac{1}{4}(x_1^4 + x_2^2 + 2x_4),$$

Table 3. 23 *rotationally non-equivalent and translationally non-related configuration symbols in the UUDD ring*

A A A A	*A A C C*	*A C A B*	*A C A D*
A A A B	*A C A C*	*A A B D*	*A B B C*
A A A C	*A A D D*	*A A D B*	*A C B B*
A A A D	*A D A D*	*A B A D*	*A B C D*
A A B B	*A A B C*	*A A C D*	*A D C B*
A B A B	*A A C B*	*A A D C*	

and the figure counting series $e(u, v) = u + v$, so

$$Z(C_4, 1 + u) = 1 + u + 2u^2 + u^3 + u^4,$$

from which the following six rotationally non-equivalent patterns can be immediately written down:

AAAA, *AAAB*, *AABB*, *ABAB*, *ABBB*, *BBBB*.

Mapping of X into R in deriving the translationally non-related patterns can be expressed as

$$\varphi_{\mathbf{t}_1/2} = \begin{pmatrix} a & b & c & d \\ r^1 & r^1 & r^1 & r^1 \end{pmatrix}, \quad \varphi_{\mathbf{t}_2/2} = \begin{pmatrix} a & b & c & d \\ r^1 & r^1 & r^1 & r^1 \end{pmatrix},$$

$$\varphi_{(\mathbf{t}_1+\mathbf{t}_2)/2} = \begin{pmatrix} a & b & c & d \\ r^0 & r^0 & r^0 & r^0 \end{pmatrix},$$

where

$$r^0 = \begin{pmatrix} A & B \\ A & B \end{pmatrix} \quad \text{and} \quad r^1 = \begin{pmatrix} A & B \\ B & A \end{pmatrix}.$$

The relations are shown in Table 4(*a*), from which the two translationally related pairs can be derived:

AAAA and *BBBB*, *AAAB* and *ABBB*.

These two pairs are also in the enantiomorphic relation, so the total number of independent patterns is four, all of which are shown in Fig. 8.

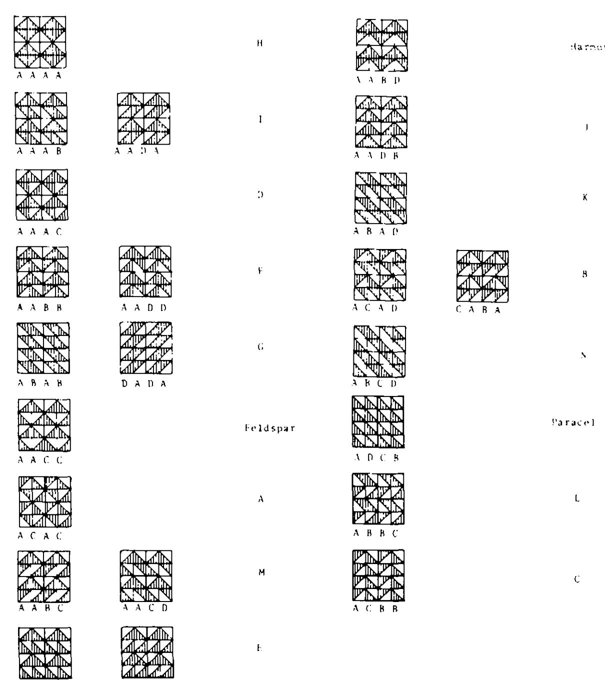


Fig. 6. 17 possible configuration patterns and their notation symbols in the *UUDD* ring. Enantiomorphic patterns are paired together. These are all composite, constructed from four unit patterns. Smith & Rinaldi (1962) notation is also shown.

Configurations based on the *UUUD* ring

The number of possible tile orientations in one box is the same as in the *UUDD* ring [Fig. 7(*b*)]. Hence the number and the notation symbols of both rotationally non-equivalent and translationally non-related patterns are exactly the same for the *UUDD* ring. In this case, however, mapping of X into R in the enantiomorphic operation can be expressed as

$$\varphi_{\rm E} = \begin{pmatrix} a\,b\,c\,d \\ r\,r\,r\,r \end{pmatrix}, \quad \text{where } r = \begin{pmatrix} A\ B\ C\ D \\ D\ C\ B\ A \end{pmatrix}.$$

Table 4. *Derivation tables for translationally related symbols in the UDUD ring and enantiomorphic ones in the UUUD ring*

(*a*) Translationally related

	$\mathbf{t}_1/2$	$\mathbf{t}_2/2$	$(\mathbf{t}_1+\mathbf{t}_2)/2$
	a b c d	*a b c d*	*a b c d*
A	*B B B B*	*B B B B*	*A A A A*
B	*A A A A*	*A A A A*	*B B B B*
	2 1 4 3	4 3 2 1	3 4 2 1

(*b*) Enantiomorphic

	a b c d
A	*D D D D*
B	*C C C C*
C	*B B B B*
D	*A A A A*
	2 1 4 3

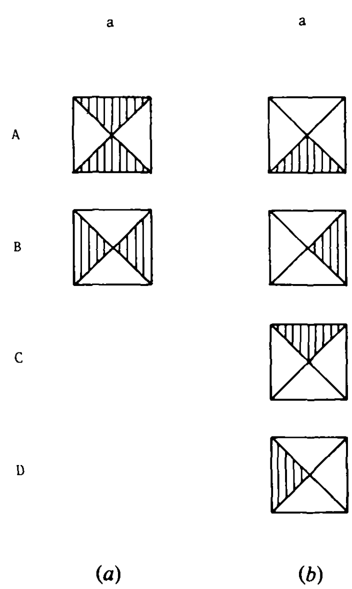


Fig. 7. (*a*) Two different tile orientations (*A*,*B*) in one box, *a*, in the *UDUD* ring. (*b*) Four different tile orientations (*A*,*B*,*C*,*D*) in one box, *a*, in the *UUUD* ring.

The relations are shown in Table 4(*b*), from which the following seven enantiomorphic patterns can be easily derived:

AAAA and *DDDD*, *AAAB* and *DDCD*, *AAAD* and *DDAC*, *AABC* and *DDBC*, *AACB* and *DDCB*, *AABD* and *DDAC*, *AADB* and *DDCA*.

Therefore the total number of independent patterns is 16 (=23 − 7), all of which are shown in Fig. 9.

Conclusion

The above systematic derivation has disclosed that there are 17 different configurations (including six enantiomorphic) in the *UUDD* ring, four different ones (two enantiomorphic) in the *UDUD* ring, and 16 different ones (seven enantiomorphic) in the *UUUD*

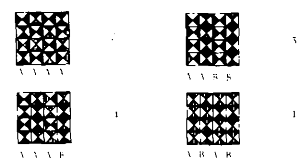


Fig. 8. Four possible configuration patterns and their symbol notations in the *UDUD* ring. Smith & Rinaldi (1962) notation is also shown.

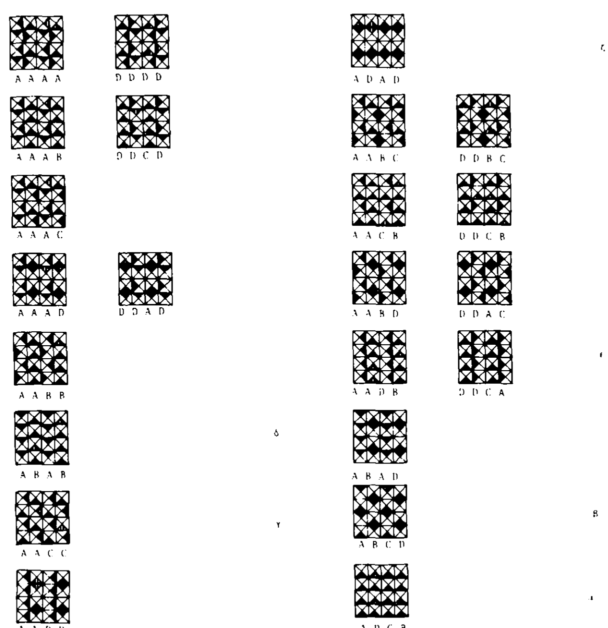


Fig. 9. 16 possible configuration patterns and their symbol notations in the *UUUD* ring. Enantiomorphic patterns are paired together. Smith & Rinaldi (1962) notation is also shown.

ring. The results have contained not only all the configurations presented by Smith & Rinaldi (1962), but also some other possibilities not predicted by them, especially in the *UUUD* ring.

The derivation procedure mentioned here is completed by the symbol operation only, without treating any real or symbolized configuration models. Therefore, starting tile orientations different from those used here might lead to different patterns from those mentioned, but the number and the kinds of symbol notations for derived configurations are invariant.

The new notation system is so simple and so faithful to the structure that it is now very easy to draw out or recall the corresponding configuration from the given symbol only.

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Propriétés des Réseaux de Coïncidence et DSC

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Abstract

Coincidence-site lattices and pattern-shift lattices (DSC) are of importance in the structural model of grain boundaries and crystalline interfaces. If two lattices can be represented by two Poisson distributions, the scalar product and the convolution product of these two functions allow the respective definitions of the coincidence-site lattice and the DSC lattice associated with these two lattices. These two operations are associative and commutative. After specification of the conditions in which they are also distributive, it is shown that this approach allows generalization of the twin-product notion and indicates the relationships between coincidence-site and DSC lattices, in particular for cubic lattices.

Introduction

Les réseaux de coïncidence et DSC* jouent un rôle important dans le modèle géometrique des joints de grains et des interfaces cristallines. L'étude de ces réseaux et de certaines de leurs propriétés, en particulier à partir de la théorie des nombres et de la théorie des groupes, a fait l'objet de nombreuses publications (Woirgard & de Fouquet, 1972; Pumphrey & Bowkett, 1972; Ishida & McLean, 1973, 1974; Fortes, 1973, 1974; Grimmer, Bollmann & Warrington, 1974; Warrington & Grimmer, 1974; Grimmer, 1974*a*,*b*; Iwasaki, 1976).

* Le sigle DSC ou DSCL vient de l'anglais Displacement Shift Complete Lattice.

Il est possible d'aborder ces problèmes à partir de la représentation d'un réseau $\mathscr{r}$ par une distribution de Poisson; soit

$$\mathscr{r} = \sum_m \sum_n \sum_p \delta(\mathbf{r} - m\mathbf{a}_1 - n\mathbf{a}_2 - p\mathbf{a}_3). \qquad (1)$$

Dans cette expression m, n, p sont des entiers positifs ou négatifs, $\mathbf{a}_1$, $\mathbf{a}_2$, $\mathbf{a}_3$ sont des vecteurs définissant une maille primitive du réseau $\mathscr{r}$ dont chaque point est représenté par une fonction $\delta_{mnp}(\mathbf{r})$ locale.

Après avoir montré que les réseaux de coïncidence et DSC peuvent se définir respectivement à partir du produit scalaire et du produit de convolution de distributions de Poisson, nous étudierons des exemples de propriétés de ces réseaux, en particulier dans le système cubique.

Représentation algébrique des réseaux de coïncidence et DSC

Dans ce qui suit, nous nous placerons dans l'espace euclidien à trois dimensions et nous adopterons les notations suivantes: les lettres minuscules seront utilisées pour nommer des réseaux (ou les fonctions associées à ces réseaux) de l'espace direct, les lettres majuscules pour des réseaux de l'espace réciproque; ainsi, $\mathscr{r}_\alpha$ et $\mathscr{r}_\beta$ représenteront les réseaux α et β, $\mathscr{R}_\alpha$ et $\mathscr{R}_\beta$ leur réseau réciproque respectif, $\mathscr{c}_{\alpha\beta}$ le réseau de coïncidence et $\mathscr{d}_{\alpha\beta}$ le réseau DSC construits sur $\mathscr{r}_\alpha$ et $\mathscr{r}_\beta$, $\mathscr{C}_{\alpha\beta}$ le réseau de coïncidence et $\mathscr{D}_{\alpha\beta}$ le réseau DSC construits sur $\mathscr{R}_\alpha$ et $\mathscr{R}_\beta$. De plus le passage de l'espace

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