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Topological Approach to the Niggli Lattice Characters

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Abstract

The way in which Niggli characters are introduced nowadays is not very satisfying. In this paper a more exact abstract method based on topological concepts is proposed. Any lattice can be represented by a point in E_5, its Niggli point. Then to any system of lattices there corresponds a set of points in E_5 called the image of this system. A Bravais type is taken formally as a system of all lattices of this type. The same can be done with the Niggli characters. The main result is: The image of a Niggli character is a component (*i.e.* a maximum connected subset) of the image of that Bravais type which contains the character. The image of any Niggli character is a convex set. This enables a simple physical (dynamical) interpretation. Since the decomposition of a set in E_5 into components is unique it can be used conversely for definition of the Niggli characters.

Introduction

The Niggli lattice characters* (Niggli, 1928; Mighell, Santoro & Donnay, 1969; de Wolff, 1983) are used to introduce a finer division of lattices than the commonly used Bravais types. It is not the only attempt that has been made. Most readers are acquainted with the method of Delaunay (1933) used in the old editions of *International Tables for X-ray Crystallography* (1952) for determining the Bravais type of a lattice. The criterion here is the shape of the Voronoi domain. The table constructed by Delaunay distinguishes 24 cases giving a division of lattices into 24 *Symmetriesorten.* This is a subdivision of the Bravais types, the *hR*, *tI*, *oI* and *mI* lattices being further divided according to special relations between the parameters of their conventional cells. The Delaunay procedure is elegant though not very quick and has experienced a revival thanks to Burzlaff & Zimmermann (1985) who have written a computer program *DELOS* (Zimmermann & Burzlaff, 1985) which is based on this procedure.

From a quite different angle the problem has been studied by Schwarzenberger (1972). His approach is abstract and requires a considerable knowledge of topology. In principle (and in short), he works with the sets of all lattices, all primitive bases and all reduced bases making them (after some identifications) topological spaces. This is done by means of a map from the general linear group. General considerations are carried out in n dimensions and detailed results gained for $n = 1, 2, 3$. They are illustrated by instructive figures. In this classification, the *tP*, *tI* and *oC* lattices are further divided.

The present *International Tables for Crystallography* (1987) use for determining the Bravais type a method suggested by Niggli (1928) which has its roots in the reduction theory of the positive-definite quadratic forms. It divides lattices into 44 classes called characters which can be described by special relations between the shortest vectors. Thus they are more freely related to the symmetry of the lattice, forming nevertheless a subdivision of the Bravais types.

Each of the three mentioned classifications is based on different principles. Therefore, their convenience and applicability to various tasks are different. It is not the aim of this paper to compare their particular advantages and disadvantages and to study their intrinsic relationships. Here we are interested only in one of these classifications, the Niggli characters.

* Also called 'lattice characters' or 'Niggli characters' or simply 'characters'.

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They attracted our attention because of the disturbing fact that until now they have not been introduced in a reliable and mathematically exact way.

To divide a set into classes requires first the choice of a criterion according to which this division ought to be made. Let us look more closely at the Niggli characters from this point of view.

There is no difficulty in determining the Niggli character of a given lattice. We simply take the Niggli table (*e.g.* Mighell *et al.*, 1969; de Wolff, 1983)* and compare the parameters of the Niggli cell of the lattice with the entries of this table. The table was constructed for the primary purpose of determining the Bravais type of a lattice: to every entry of the table there belongs exactly one Bravais type. Since there are 44 entries and only 14 Bravais types it follows that some of the Bravais types must occur in the table more than once. Niggli used this opportunity to divide the Bravais types into finer classes, now called lattice characters (de Wolff, 1983).

From a pure logical standpoint, there can be no objections. To any lattice there is attached a unique character (denoted by a positive integer not greater than 44) and all lattices of the same character belong to the same Bravais type. Also, the practical procedure of how to determine the character of a given lattice is simple and straightforward.

Less satisfactory, however, is the question of a general definition of the characters. It is clear that we would like to know their factual meaning or, in other words, what two lattices of the same character have in common.

Here we are on shaky ground. Niggli expresses himself in a descriptive rather than a formally rigorous way, perhaps because he was preparing an extensive account (Niggli, 1928, p. 115) for *Z. Kristallogr.* which, however, as far as we could discover, did not appear. Thus it is sometimes difficult to decide absolutely according to the Niggli criterion (Niggli, 1928, p. 114; de Wolff, 1988) whether two lattices have the same character or not.

The greatest attention was given to this problem by P. M. de Wolff who has analysed it very thoroughly in several papers (de Wolff, 1983, 1988; de Wolff & Gruber, 1991), perhaps from all possible aspects. And if he comes to the conclusion (1988) that 'so far there does not exist an exact general definition' and that 'regarded as a concept (rather than a list of explicit criteria for each of the 44 characters) the lattice character so far has not been defined as clearly as the Bravais types and systems', we can only agree with him.

On the other hand, we are bound to say that de Wolff (1983, p. 744; 1988) has presented an alternative definition based on a lattice deformation which is continuous in the parameters

$$A, B, C, D, E, F.* \qquad (1)$$

This definition is exact and concise and we shall meet it in the final section. It is somewhat surprising that he does not put a greater emphasis on it. Perhaps it is because the definition seems to him (1988) to 'lack a simple interpretation' and not 'to be easily applicable' which is, of course, correct. He also in no way suggests how to verify the equivalence of the two definitions.

With this exception, the present state of affairs may leave us with an uncomfortable impression that the whole thing is not exactly up to date and deserves, perhaps, to be 'modernized'. It is the aim of this paper to show that it can be done effectively with basic topological concepts. Moreover, this method enables a mathematically rigorous treatment of the matter.

The clue was found in an idea which associates any lattice with a point in the five-dimensional Euclidean space E_5. This can be done in various ways.† Here this point is derived from the Niggli cell and called therefore the Niggli point of the lattice.

The idea of applying E_5 was suggested by Burzlaff & Zimmermann (1985). However, they took advantage of it only in a limited form using the three-dimensional space E_3 for lattices of at least monoclinic symmetry. On the other hand, this restriction enabled them to visualize the results directly in figures. Also, topological methods are not new in this field. They are employed in the paper by Schwarzenberger (1972) and, implicitly, also in that by Burzlaff & Zimmermann (1985).

Here we move freely in five dimensions following thus Wondratschek (1986) who is applying this method to a similar problem. For our purposes the space E_5 is very appropriate. Five dimensions are enough since we are interested only in the 'shape' of the lattice and not in its 'size'. Further, the problem becomes 'homogeneous' in all the parameters (1) where hitherto the A, B, C were looked upon differently from the D, E, F.

Thus, to any system $\mathscr{S}$ of lattices there corresponds a set of points in E_5 called the image of this system. Conversely, to any set of Niggli points in E_5 there belongs a system $\mathscr{S}$ of lattices. Consequently, any division of the system $\mathscr{S}$ is transferred to E_5 as a division of its image and any division of this image

* More detailed references can be found in the following section.

* The current notation $A=\mathbf{a}\cdot\mathbf{a}$, $B=\mathbf{b}\cdot\mathbf{b}$, $C=\mathbf{c}\cdot\mathbf{c}$, $D=\mathbf{b}\cdot\mathbf{c}$, $E=\mathbf{c}\cdot\mathbf{a}$, $F=\mathbf{a}\cdot\mathbf{b}$ is used throughout, the vectors **a**, **b**, **c** relating usually to the Niggli cell in a normalized description.

† For example, a referee of this paper has shown a very elegant way to use the Delaunay procedure for this purpose. However, this would lead us to regions in E_5 which are too far from our interest since 'the comparison between the Niggli and the Delaunay classification shows rather low correlation' (Burzlaff & Zimmermann, 1985).

induces a division of the system $\mathscr{S}$.* We shall use both these 'directions' but the latter will be of greater importance for us since the sets in E_5 can be viewed from various diverse aspects.

Raised in this way into five-dimensional space our problem suddenly becomes clear. It turns out that the crucial concept relating to the Niggli characters is the connectedness. In particular, we shall use the fact that in a topological space (here in E_5) any set can be divided in a unique way into so-called components, that is into connected subsets which cannot be enlarged without ceasing to be connected.

Thus we shall proceed in the following way: (i) we divide all lattices into Bravais types; (ii) we construct the images of the Bravais types; (iii) we divide any image into components; (iv) we transfer these divisions back to the Bravais types and (v) we obtain - with some surprise - the lattice characters.

This is the general common principle we were looking for: the images of the Niggli characters are simply components of the images of the Bravais types. On the basis of this principle the Niggli characters can be defined in an abstract and mathematically exact way.

Whether Niggli himself suspected something of this kind cannot be guessed, but his insight must be admired.

Explicit description of the Niggli characters

The system of all three-dimensional lattices is denoted $\mathscr{B}$. We introduce the 'reduced'† parameters

$$u=\mathbf{a}^2/\mathbf{c}^2, \qquad v=\mathbf{b}^2/\mathbf{c}^2,$$
$$x=2\mathbf{b}\cdot\mathbf{c}/\mathbf{c}^2, \qquad y=2\mathbf{c}\cdot\mathbf{a}/\mathbf{c}^2, \qquad z=2\mathbf{a}\cdot\mathbf{b}/\mathbf{c}^2$$

for a cell C‡ described by the vectors $\mathbf{a}, \mathbf{b}, \mathbf{c}$. These vectors can always be chosen in such a way that

$$u\le v\le 1,$$
$$\text{if } u=v \text{ then } |x|\le|y|,$$
$$\text{if } v=1 \text{ then } |y|\le|z|,$$
$$\text{either } x>0,\ y>0,\ z>0 \qquad (2)$$
$$\text{or } x\le 0,\ y\le 0,\ z\le 0. \qquad (3)$$

In this case we speak about a normalized description

$$u, v, x, y, z \qquad (4)$$

of C. Such a description is unique. Further, we shall use only normalized descriptions of cells without saying it explicitly. We distinguish between positive and non-positive cells according to whether (2) or (3) is true.

* A more accurate explanation is given in the next section.

† We use the inverted commas to avoid a confusion of these parameters with the current parameters of a reduced cell.

‡ Only primitive cells are admitted.

In any lattice there is a unique cell, called the Niggli cell, which is conventionally taken for representing the lattice. This cell minimizes the sum $a+b+c$ fulfilling besides a system of inequalities which guarantee its uniqueness (de Wolff, 1983, § 9.3.2). Thus, if we take for a lattice L its Niggli cell and describe it in a normalized way we get a unique point

$$[u, v, x, y, z] \qquad (5)$$

which is called the Niggli point of the lattice L. The set of Niggli points of all possible lattices is denoted Π.

Any Niggli point belongs either to the five-dimensional polyhedron

$$\Omega^+:\ u\le v\le 1, \qquad 0\le x\le v, \quad 0\le y\le u, \quad 0\le z\le u \qquad (6)$$

or to the polyhedron

$$\Omega^-:\ u\le v\le 1, \quad 0\le u+v+x+y+z, \qquad -v\le x\le 0, \quad -u\le y\le 0, \quad -u\le z\le 0. \qquad (7)$$

The relationships between these sets are as follows:

$$\Pi\subset\Omega^+\cup\Omega^-\subset E_5,$$
$$\Pi\ne\Omega^+\cup\Omega^-, \qquad \Omega^+\cap\Omega^-\ne\varnothing.$$

Two lattices have the same Niggli point if and only if they are geometrically similar. Thus, if (5) is a Niggli point there exists an infinite number of lattices for which (5) has this property. Since all these lattices are geometrically similar we need not (with regard to the aim of this paper) distinguish between them and can consider the just-established correspondence between the sets $\mathscr{B}$ and Π as one-to-one.

We start with the generally used division of lattices into 14 classes called the Bravais types.* For these types the symbols

$$cP, cI, cF, hP, hR, tP, tI,$$
$$oP, oC, oI, oF, mP, mC, aP$$

are used (*International Tables for X-ray Crystallography*, 1969). For a general Bravais type which has no other specification, we use the symbol xY. The set of the Niggli points of all lattices of the Bravais type xY is denoted $\{xY\}$ and called the image of this Bravais type.

The classes of the Niggli division are called characters. Since any character is part of a Bravais type, all lattices of the same character belong to the same Bravais type. Also, the Niggli cells of lattices of the same character are either all positive or all non-positive. Thus we can speak about positive and non-positive Niggli characters.

There are altogether 44 Niggli characters which are thus on the average three times finer than the Bravais

* Thus a Bravais type is formally a subset of $\mathscr{B}$.

types. However, the way in which the particular Bravais types are divided into characters is not 'uniform' and some of them are not divided at all.

The Niggli character of a given lattice can be determined by the Niggli table. This table has been through several developments. Paradoxically, Niggli (1928) himself did not establish a table, he just made a detailed analysis richly illustrated by a series of figures. Only by means of the numbers of these figures could the particular characters be referred to. Later, Mighell *et al.* (1969) arranged the characters into a real table, each entry becoming a current number. This number is also used for denoting the character determined by this entry. Some corrections and modifications were incorporated by Mighell & Rodgers (1980). The improved version by de Wolff (1983) is graphically simpler but the main improvement is in changing the order of the entries whose numbers, however, remained the same. In this way he obtained a 'first-hit' sequence where the first agreement with the given data determines the correct character. This was not always the case in the previous tables. Finally, in the Appendix of this paper there is a modification of the Niggli table for the 'reduced' parameters (4). It has a particularly simple appearance.

From the present notation of a Niggli character by a mere integer k ($1 \le k \le 44$), the Bravais type of the lattice is not apparent unless the Niggli table is at hand. This is often inconvenient and therefore we use here a more explicit symbol $xY.k$ showing both the Bravais type xY and the number k of the character. The set of Niggli points of all lattices of the Niggli character $xY.k$ is denoted $\{xY.k\}$ and called the image of this character.

For example,

$$oI.8,\ oI.19,\ oI.42$$

are all Niggli characters which contain lattices of the Bravais type oI. Thus,

$$\{oI\} = \{oI.8\} \cup \{oI.19\} \cup \{oI.42\},$$

$$\{oI.8\} \cap \{oI.19\} = \{oI.8\} \cap \{oI.42\}$$
$$= \{oI.19\} \cap \{oI.42\} = \varnothing.$$

The two divisions of lattices which we have just described generate two divisions of the set Π, namely the images of the Bravais types and the images of the Niggli characters, the latter being a subdivision of the former. What do these images look like?

Viewing E_5 as a Euclidean space and using the possibilities which this concept offers, we soon observe (see Table 1) that the 'geometrical' shape of the images $\{xY.k\}$ and their mutual relationships are fairly complicated. These sets are composed of certain parts of various-dimensional 'faces'* of the polyhedra

* Added must be the interiors of Ω^+ and Ω^-.

Table 1. *Explicit descriptions of the Niggli characters*

(*a*) Positive Niggli characters

Character	$u \sim v$	$v \sim 1$	$0 \sim x$	$x \sim v$	$0 \sim y$	$y \sim u$	$0 \sim z$	$z \sim u$	Condition
$cF.1$	=	=		=		=		=	
$hR.2$	=	=	<	<					$x = y = z$
$hR.9$	=	<	<	=		=		=	
$tI.18$	≤	=	<			=		=	$y = 2x$
$oI.19$	≤	=		≤	<	=		=	$y < 2x$, $x + y < 2$
$oF.26$	≤	<	<			=		=	$y = 2x$
$mC.10$	=	<	<	≤			<	≤	$x = y$, $y + z < 2u$
or	=	=	<					≤	$x = y < z$
$mC.20$	<	=	<	≤	<	<			$y = z$
or	=	=	<					<	$x < y = z$
$mC.27$	≤	<		≤	<	=		=	$y < 2x$, $x + y < 2v$
$mC.28$	≤	<				=	<	<	$z = 2x$
$mC.29$	≤	≤			<	<		=	$y = 2x$
$mC.30$	<	≤		=			<	≤	$z = 2y$
$aP.31$	<	<	<	<	<	<	<	<	
or	<	<		=		≤	<	≤	$z < 2y$, $y + z < 2u$
or	<	≤		<	<	<		=	$y < 2x$
or	<	=	<	<	<			<	$y < z$
or	<	=		=				≤	$y < z < 2y$
or	≤	<		<		=	<	<	$z < 2x$
or	=	<	<			<	<	<	$x < y$
or	=	≤				<		=	$x < y < 2x$
or	=	=	<					<	$x < y < z$

(*b*) Non-positive Niggli characters
Notation: $s = u + v + x + y + z$

Character	$u \sim v$	$v \sim 1$	$-v \sim x$	$x \sim 0$	$-u \sim y$	$y \sim 0$	$-u \sim z$	$z \sim 0$	$0 \sim s$	Condition
$cP.3$	=	=		=		=		=		
$cI.5$	=	=							=	$z = y = x$
$hP.12$	=	≤		=		=	=	<		
$hP.22$	<	=	=		<	=		=		
$hR.4$	=	=		<					<	$z = y = x$
$hR.24$	<	=				<			=	$z = y$, $u + y = v + x$
$tP.11$	=	<	<	=		=		=		
$tP.21$	<	=		=	<	=		=		
$tI.6$	=	=					<		=	$z < y = x$
$tI.7$	=	=		<					=	$z = y < x$
$tI.15$	=	<	=	<	=			=		
$oP.32$	<	<		=	<	=		=		
$oC.13$	=	≤		=		=	<	<		
$oC.23$	<	=	<	<	<	=		=		
$oC.36$	≤	<		=	=	<		=		
$oC.38$	<	≤		=	<	=	=			
$oC.40$	<	<	=		<	=		=		
$oI.8$	=	=					<		=	$z < y < x$
$oI.42$	<	<	=		=	<		=		
$oF.16$	=	<					<	<	=	$y = x$
$mP.33$	≤	<		=	<	<		=		
$mP.34$	<	≤		=		=	<	<		
$mP.35$	<	<	<	<	<	=		=		
$mC.14$	=	<		<			<	≤	<	$y = x$
or	=	=		<			<		<	$z < y = x$
$mC.17$	=	<			<		<		=	$y < x$
$mC.25$	<	=	<	≤	<	<			<	$z = y$
or	<	=			<				=	$z = y$, $u + y < v + x$
or	=	=		≤					<	$z = y < x$
$mC.37$	≤	<	<	<	=	<		=		
$mC.39$	<	≤	<	<	<	=	=			
$mC.41$	<	<	=		<	<		=		
$mC.43$	<	<					<	<	=	$u + y = v + x$
or	<	=					<		=	$z < y$, $u + y = v + x$

Table 1(*b*) (*cont.*)

Character	$u \sim v$	$v \sim 1$	$-v \sim x$	$x \sim 0$	$-u \sim y$	$y \sim 0$	$-u \sim z$	$z \sim 0$	$0 \sim s$	Condition
aP.44	$<$	$<$	$<$	$<$	$<$	$<$	$<$	$<$	$<$	
or	$<$	$<$	$<$	$<$	$<$	$<$		$=$		
or	$<$	$<$			$<$		$<$		$=$	$u+y<v+x$
or	$<$	$\le$	$<$	$<$		$=$	$<$	$<$		
or	$<$	$=$	$<$	$<$		$<$	$<$		$<$	$z<y$
or	$<$	$=$					$<$		$=$	$z<y$, $u+y<v+x$
or	$\le$	$<$		$=$	$<$	$<$	$<$	$<$		
or	$\le$	$=$		$=$		$<$	$<$			$z<y$
or	$=$	$<$		$<$	$<$		$<$	$<$	$<$	$y<x$
or	$=$	$<$		$<$	$<$			$=$		$y<x$
or	$=$	$=$		$<$			$<$		$<$	$z<y<x$

Ω^+ and Ω^- and are quite irregularly distributed along the boundary of these polyhedra. From this point of view the sets $\{xY.k\}$ are not the object of our interest here.

However, by considering E_5 merely a metric or topological space, we get a different impression. It turns out that the sets $\{xY.k\}$ and especially their systems

$$\{xY.k\}, \{xY.l\}, \ldots, \{xY.s\} \tag{8}$$

which constitute the complete image $\{xY\}$ possess very expressive topological properties which characterize them in such a strong way that they can be used for a definition of the system (8), a definition which is based solely on the set $\{xY\}$ and not on the Niggli characters

$$xY.k, xY.l, \ldots, xY.s.$$

This has profound consequences. It enables one to introduce the Niggli characters independently of the Niggli table by using only the topological properties of the sets $\{xY\}$. In this way, the Niggli characters will gain an exact abstract meaning.

To prove (and formulate properly) all these statements is our next task. To fulfil it we must first have an exact knowledge of the images $\{xY.k\}$ of all 44 Niggli characters. This knowledge may be gained from Table 1 which gives an explicit description of these sets.

Table 1(a) relates to the positive characters, Table 1(b) to the non-positive. In the first column are given the symbols $xY.k$ of the lattice characters (although, actually, their images are concerned). In both tables the lattice characters are grouped according to the corresponding Bravais types. The concise form of the tables is enabled by the inequalities (6) and (7). Special conditions, if necessary, are added in the last column. The blank spaces are ignored.* Any entry may be directly checked by the Niggli table. Not so straightforward is the question of the completeness of Table 1. This requires the knowledge of the fairly complicated shape of the set Π (Gruber, 1978).

Example: According to Table 1(a) the image $\{mC.20\}$ of the Niggli character $mC.20$ is the set of points (5) fulfilling either $0<x\le 1$, $0<y=z<u<v=1$ or $0<x<y=z<u=v=1$.

Before stating our main results we shall insert a brief summary of the concepts and statements from topology which will be needed.

Auxiliary concepts and statements from topology

Here we move in the space E_r $(r \ge 1)$ which is provided with the Euclidean metric ρ. Since the whole section is meant to be a summary of the basic topological knowledge, the statements (with one exception which is formulated specially for our purposes) are given without proofs.

The points of E_r are usually denoted $X, Y, \ldots$, the subsets $\mathbf{M}, \mathbf{N}, \ldots$. The distance $\rho(X, \mathbf{M})$ of a point X from a set $\mathbf{M}$ is the infimum of the numbers $\rho(X, Y)$ where $Y \in \mathbf{M}$. If $X \in \mathbf{M}$ then obviously

$$\rho(X, \mathbf{M}) = 0. \tag{9}$$

However, (9) may be true also for a point X which does not belong to $\mathbf{M}$. The set of points X fulfilling (9) is denoted $\bar{\mathbf{M}}$ and called the closure of the set $\mathbf{M}$. It fulfils

$$\overline{\mathbf{M} \cup \mathbf{N}} = \bar{\mathbf{M}} \cup \bar{\mathbf{N}}. \tag{10}$$

We say that the sets $\mathbf{M}, \mathbf{N}$ are separated if any point of $\mathbf{M}$ has a positive distance from $\mathbf{N}$ and any point of $\mathbf{N}$ a positive distance from $\mathbf{M}$. In a more formal way, $\mathbf{M}$ and $\mathbf{N}$ are separated if

$$\mathbf{M} \cap \bar{\mathbf{N}} = \mathbf{N} \cap \bar{\mathbf{M}} = \varnothing.$$

Two separated sets are disjoint but two disjoint sets need not be separated.

(*Example*. In E_1 let $\mathbf{M}_1, \mathbf{M}_2, \mathbf{N}_1, \mathbf{N}_2$ be the sets of real numbers x fulfilling $x<0$, $x\le 0$, $0<x$, $0\le x$, respectively. Then

$\mathbf{M}_1, \mathbf{N}_1$ are disjoint and separated,

$\left.\begin{matrix}\mathbf{M}_1, \mathbf{N}_2 \\ \mathbf{M}_2, \mathbf{N}_1\end{matrix}\right\}$ are disjoint and not separated,

$\mathbf{M}_2, \mathbf{N}_2$ are not disjoint and not separated.)

A non-empty set $\mathbf{M}$ is called connected if it cannot be considered a union of two non-empty separated sets. (*Example*: In E_1 the set of all real numbers x fulfilling $0<|x|$ is not connected.)

The union of two connected sets which have a common point is connected. Any linear interval is a connected set. If f is a continuous mapping of a connected set $\mathbf{Q} \subset E_q$ $(q \ge 1)$ into E_r then $f(\mathbf{Q})$ is connected. If in particular the set $\mathbf{Q}$ is a closed linear interval, the set $f(\mathbf{Q})$ is called a path. Thus a

* In any of these spaces, $=$, $<$ or $\le$ may be placed which, however, is superfluous for the description of the set $\{xY.k\}$.

path is a connected set. We say that the points X, Y are connected by the path $\mathbf{P}$ if $X, Y \in \mathbf{P}$.

A set $\mathbf{M}$ may have various connected subsets. Among them those which are 'maximum' sets with this property are of special importance. They are called components of the set $\mathbf{M}$. More precisely, we say that $\mathbf{C}$ is a component of the set $\mathbf{M} = \varnothing$ if (i) $\mathbf{C} \subset \mathbf{M}$, (ii) $\mathbf{C}$ is connected, (iii) if $\mathbf{C} \subset \mathbf{N} \subset \mathbf{M}$, $\mathbf{C} \neq \mathbf{N}$ then $\mathbf{N}$ is not connected.

Any point X of a set $\mathbf{M}$ belongs to a component of $\mathbf{M}$. This component is the union of all connected subsets of $\mathbf{M}$ which contain X. If $\mathbf{C}_1, \mathbf{C}_2$ are components of $\mathbf{M}$ then they are either identical or separated (and therefore disjoint). This means that the system $\mathscr{C}$ of all components of $\mathbf{M}$ stands for a decomposition of the set $\mathbf{M}$ into connected classes such that any two of them are separated. This statement, which is not difficult to prove, can be to a certain extent inverted. This inversion has a crucial meaning for our reasonings.

Proposition 1. Let

$$\mathbf{M}_1, \ldots, \mathbf{M}_s \ (s \geq 1) \tag{11}$$

be a decomposition of a set $\mathbf{M}$ ($\mathbf{M} \neq \varnothing$) into a finite number of classes.* Let any class $\mathbf{M}_i$ $(1 \leq i \leq s)$ be connected and any two classes $\mathbf{M}_i, \mathbf{M}_j$ $(1 \leq i < j \leq s)$ separated. Then (11) stands for the system of all components of the set $\mathbf{M}$.

Proof of proposition 1. The matter is clear for $s = 1$. Let $s > 1$. Denote by $\mathscr{M}$ the system (11) and by $\mathscr{C}$ the system of all components of $\mathbf{M}$.† We want to prove

$$\mathscr{M} = \mathscr{C}. \tag{12}$$

Two lemmas will help us to do this.

Lemma 1. For any $\mathbf{C} \in \mathscr{C}$ there exists such $\mathbf{M}_q \in \mathscr{M}$ that $\mathbf{C} \subset \mathbf{M}_q$.

Proof of lemma 1. Suppose the opposite is true so that such points $X, Y \in \mathbf{C}$ exist which belong to different classes of $\mathscr{M}$. Without loss of generality we may assume $X \in \mathbf{M}_1$. Then $Y \in \mathbf{M}'$ where

$$\mathbf{M}' = \mathbf{M}_2 \cup \ldots \cup \mathbf{M}_s.$$

Any point of $\mathbf{M}_1$ has a positive distance from any of the sets

$$\mathbf{M}_2, \ldots, \mathbf{M}_s \tag{13}$$

and thus also a positive distance from $\mathbf{M}'$. On the other hand, any point of $\mathbf{M}'$ has [as a point of one of the sets (13)] a positive distance from $\mathbf{M}_1$. This means that $\mathbf{M}_1, \mathbf{M}'$ are separated. Then also the sets

$$\mathbf{M}_1 \cap \mathbf{C}, \qquad \mathbf{M}' \cap \mathbf{C}$$

are separated. They are not empty (the first containing the point X and the second the point Y) and their union is the set $\mathbf{C}$. This, however, does not agree with the fact that $\mathbf{C}$ as a component is connected.

Lemma 2. If $\mathbf{M}_p \in \mathscr{M}$, $\mathbf{C} \in \mathscr{C}$, $\mathbf{M}_p \cap \mathbf{C} \neq \varnothing$ then $\mathbf{M}_p = \mathbf{C}$.

Proof of lemma 2. Let X be a common point of $\mathbf{M}_p$ and $\mathbf{C}$. Since $\mathbf{C}$ is the union of all connected subsets of $\mathbf{M}$ containing the point X, $\mathbf{M}_p \subset \mathbf{C}$. According to lemma 1 such $\mathbf{M}_q \in \mathscr{M}$ may be found that $\mathbf{C} \subset \mathbf{M}_q$. Thus, $\mathbf{M}_p \subset \mathbf{M}_q$. But $\mathbf{M}_p, \mathbf{M}_q$ are classes of a decomposition of $\mathbf{M}$. Consequently, $\mathbf{M}_p = \mathbf{M}_q$ and $\mathbf{M}_p = \mathbf{C}$.

Now let us return to the proof of proposition 1.

Let $\mathbf{M}_p$ be an arbitrary element of $\mathscr{M}$. The set $\mathbf{M}_p$ being not empty contains a point X and this point X belongs to a component $\mathbf{C}$. According to lemma 2, $\mathbf{M}_p = \mathbf{C}$ so that $\mathbf{M}_p \in \mathscr{C}$ and $\mathscr{M} \subset \mathscr{C}$. Secondly, let $\mathbf{C} \in \mathscr{C}$ be an arbitrary component. It is not empty containing a point Y. Since Y belongs to $\mathbf{M}$ it must belong to one class, say $\mathbf{M}_p$, of the system $\mathscr{M}$. Applying lemma 2 again we get $\mathbf{C} = \mathbf{M}_p$ so that $\mathbf{C} \in \mathscr{M}$ and $\mathscr{C} \subset \mathscr{M}$. In this way, (12) is proved and the proof of proposition 1 completed.

Remark 1. Let us mention here the (otherwise obvious but for us vital) fact that the system of all components of a set $\mathbf{M}$ is by its definition unique and is fully determined only by the set $\mathbf{M}$ itself.

Finally, we introduce two concepts which relate to E_r as a Euclidean (not only a metric or topological) space. If X, Y are arbitrary points of E_r then the set of points

$$\lambda X + (1 - \lambda) Y \qquad (0 \leq \lambda \leq 1)$$

is denoted $\overline{XY}$ and called a straight segment with the end-points X, Y. A straight segment is a path and therefore connected.

A set $\mathbf{M} \subset E_r$ is called convex if from $X, Y \in \mathbf{M}$ it follows that $\overline{XY} \subset \mathbf{M}$. The intersection of convex sets is convex. If f is a linear mapping of a convex set $\mathbf{Q} \subset E_q$ $(q \geq 1)$ into E_r then $f(\mathbf{Q})$ is a convex set. The relationship between connectedness and convexity is simple.

Proposition 2. Any non-empty convex set is connected.

Topological properties of the sets $\{xY.k\}$

Proposition 3. For any Niggli character $xY.k$ the set $\{xY.k\}$ is convex.

Proof. Two cases will show how to proceed. First let us take the set $\{oF.16\}$. According to Table 1(b) it can be considered a set of points

$$[u, v, x, y, z] = [q, q, -p, -p, -2q + 2p] \tag{14}$$

where

$$q/2 < p < q < 1. \tag{15}$$

The two-dimensional set defined in (15) is convex

* That is, (i) $\mathbf{M}_i \neq \varnothing$ for $1 \leq i \leq s$, (ii) $\mathbf{M}_i \cap \mathbf{M}_j = \varnothing$ for $1 \leq i < j \leq s$, (iii) $\mathbf{M}_1 \cup \ldots \cup \mathbf{M}_s = \mathbf{M}$.

† The system $\mathscr{M}$ consists of s elements whereas the number of elements of $\mathscr{C}$ is not known, or even whether it is finite or infinite.

Table 2. *Relating to the proof of proposition* 3

Entry	Point	$u_i \sim v_i$	$v_i \sim 1$	$0 \sim x_i$	$x_i \sim v_i$	$0 \sim y_i$	$y_i \sim u_i$	$0 \sim z_i$	$z_i \sim u_i$	Condition
1	W_1	$<$	$=$	$<$	$=$	$<$	$<$	$<$	$\leq$	$y_1 < z_1 < 2y_1$
2	W_2	$=$	$\leq$	$<$	$<$	$<$	$<$	$<$	$=$	$x_2 < y_2 < 2x_2$
1*a*	W_1	$<$	$=$	$<$	$=$	$<$	$<$	$<$	$=$	$y_1 < 2x_1$
2*a*	W_2	$=$	$\leq$	$<$	$<$	$<$	$<$	$<$	$=$	$y_2 < 2x_2$
3*a*	W_3	$<$	$\leq$	$<$	$<$	$<$	$<$	$<$	$=$	$y_3 < 2x_3$
1*b*	W_1	$<$	$=$	$<$	$=$	$<$	$<$	$<$	$<$	$y_1 < z_1$
2*b*	W_2	$=$	$=$	$<$	$<$	$<$	$<$	$<$	$=$	$y_2 < z_2$
3*b*	W_3	$<$	$=$	$<$	$<$	$<$	$<$	$<$	$<$	$y_3 < z_3$
1*c*	W_1	$<$	$=$	$<$	$=$	$<$	$<$	$<$	$<$	
2*c*	W_2	$=$	$<$	$<$	$<$	$<$	$<$	$<$	$=$	
3*c*	W_3	$<$	$<$	$<$	$<$	$<$	$<$	$<$	$<$	

and the mapping (14) (from E_2 into E_5) is linear. Thus, $\{oF.16\}$ is convex.

Secondly, we consider $\{aP.31\}$. This is described in Table 1(a) on nine lines each line giving a subset of $\{aP.31\}$. Denote these subsets (in the given order)

$$\{aP.31\}_1, \ldots, \{aP.31\}_9$$

so that

$$\{aP.31\} = \{aP.31\}_1 \cup \ldots \cup \{aP.31\}_9 \tag{16}$$

and choose two arbitrary points $W_1, W_2 \in \{aP.31\}$. Our task is to prove that the straight segment $\overline{W_1 W_2}$ belongs to $\{aP.31\}$. The matter is clear for $W_1 = W_2$. Otherwise, we have to prove that for any λ fulfilling

$$0 < \lambda < 1 \tag{17}$$

the point

$$W_3 = \lambda W_1 + (1-\lambda) W_2$$

belongs to $\{aP.31\}$. Further, let a λ fulfilling (17) be chosen. We denote

$$W_i = [u_i, v_i, x_i, y_i, z_i] \qquad (i = 1, 2, 3)$$

so that

$$u_3 = \lambda u_1 + (1-\lambda) u_2, \ldots,$$
$$z_3 = \lambda z_1 + (1-\lambda) z_2.$$

The union in (16) shows that there are $9 \times 9 = 81$ possibilities for the positions of the points W_1, W_2. As an example we take

$$W_1 \in \{aP.31\}_5, \qquad W_2 \in \{aP.31\}_8$$

and consider Table 2. The first two entries repeat the inequalities for $\{aP.31\}_5$ and $\{aP.31\}_8$ from Table 1(a) with completed blank spaces. Further, we distinguish three cases: (a) $z_1 = u_1$, (b) $z_1 < u_1$, $v_2 = 1$, (c) $z_1 < u_1$, $v_2 < 1$. The corresponding inequalities are given in the entries 1*a*, 2*a*, 1*b*, 2*b*, 1*c*, 2*c*, where in the last column only those inequalities are given which will be needed. In particular, let us mention that, in entry 1*a*, $y_1 < z_1 = u_1 < v_1 = x_1 < 2x_1$ and, in 2*b*, $y_2 < u_2 = z_2$. Now let us take case (a), first column. From $u_1 < v_1$, $u_2 = v_2$ it follows that

$$\lambda u_1 + (1-\lambda) u_2 < \lambda v_1 + (1-\lambda) v_2,$$

that is $u_3 < v_3$ as stated in entry 3*a*. In this way Table 2 can be verified almost at first sight. Consulting finally Table 1(a) again, we find that in case (a) $Q_3 \in \{aP.31\}_3$, in case (b) $Q_3 \in \{aP.31\}_4$ and in case (c) $Q_3 \in \{aP.31\}_1$, which is $Q_3 \in \{aP.31\}$ which was to be proved. These two examples suffice to show how to complete the proof of proposition 3.

Proposition 4. For any Niggli character $xY.k$ the set $\{xY.k\}$ is connected.

Proof follows from propositions 3 and 2.

Proposition 5. Let $xY.k$, $xY.l$ be two different Niggli characters belonging to the same Bravais type xY. Then the sets $\{xY.k\}$, $\{xY.l\}$ are separated.

Proof. The idea will be seen from the following example concerning the characters $mC.10$ and $mC.20$. Here we have to prove

$$\begin{aligned} \{mC.10\} \cap \overline{\{mC.20\}} &= \varnothing, \\ \{mc.20\} \cap \overline{\{mC.10\}} &= \varnothing. \end{aligned} \tag{18}$$

Following Table 1(a), we write in a notation used in the proof of proposition 3

$$\{mC.10\} = \{mC.10\}_1 \cup \{mC.10\}_2,$$
$$\{mc.20\} = \{mC.20\}_1 \cup \{mC.20\}_2.$$

Then [with respect to (10)] the relations (18) are equivalent to

$$\left.\begin{aligned} \{mC.10\}_i \cap \overline{\{mC.20\}}_j &= \varnothing \\ \{mC.20\}_i \cap \overline{\{mC.10\}}_j &= \varnothing \end{aligned}\right. \quad (1 \leq i \leq 2, 1 \leq j \leq 2).$$

We take the case $i = j = 2$. According to Table 1(a) we can describe these sets of points as

$$\{mC.10\}_2\colon [1, 1, p, p, q], \quad 0 < p < q \leq 1,$$
$$\{mC.20\}_2\colon [1, 1, p, q, q], \quad 0 < p < q < 1.$$

The closures can be easily provided:

$$\overline{\{mC.10\}}_2\colon [1, 1, p', p', q'], \quad 0 \leq p' \leq q' \leq 1,$$
$$\overline{\{mC.20\}}_2\colon [1, 1, p', q', q'], \quad 0 \leq p' \leq q' \leq 1.$$

A point belonging simultaneously to $\{mC.10\}_2$ and $\overline{\{mC.20\}}_2$ must therefore fulfil

$$[1, 1, p, p, q] = [1, 1, p', q', q']$$

with

$$0 < p < q \leq 1, \qquad 0 \leq p' \leq q' \leq 1.$$

Such numbers p, q, p', q', however, do not exist and therefore

$$\{mC.10\}_2 \cap \overline{\{mC.20\}}_2 = \varnothing. \tag{19}$$

In a similar way,

$$\{mC.20\}_2 \cap \overline{\{mC.10\}}_2 = \varnothing. \tag{20}$$

Let us, perhaps, note that the intersection

$$\overline{\{mC.10\}}_2 \cap \overline{\{mC.20\}}_2$$

is not empty [which would immediately give both

(19) and (20)] being equal to the set of points

$$[1, 1, p, p, p], \qquad 0 \le p \le 1.$$

We can proceed like this without difficulties until the proof is completed.

Proposition 6. Let

$$xY.k, xY.l, \ldots, xY.s$$

all be Niggli characters belonging to the Bravais type xY. Then the system

$$\{xY.k\}, \{xY.l\}, \ldots, \{xY.s\}$$

stands for a decomposition of the set $\{xY\}$ into components.

Proof follows from propositions 4, 5 and 1.

Having in mind remark 1 we can now state the fundamental

Theorem 1. Let L_1, L_2 be arbitrary lattices of the same Bravais type, say xY. Then they are of the same Niggli character if and only if their Niggli points belong to the same component of the set $\{xY\}$.

Geometrical view

Here we make use of proposition 3 which has not yet been exploited.

Theorem 2. Let L_1, L_2 be arbitrary lattices. Then they are of the same Niggli character if and only if there exists a path connecting the Niggli point of L_1 with the Niggli point of L_2 such that all points of this path are Niggli points of lattices of the same Bravais type.

The condition of this theorem can be made narrower.

Theorem 3. Let L_1, L_2 be arbitrary lattices and W_1, W_2 their Niggli points. Then these lattices are of the same Niggli character if and only if all points of the straight segment $\overline{W_1W_2}$ are Niggli points of lattices of the same Bravais type.

Proofs of these two theorems will be performed simultaneously.

(i) Let L_1, L_2 be of the same Niggli character, say $xY.k$. Then W_1, $W_2 \in \{xY.k\}$. According to proposition 3 the set $\{xY.k\}$ is convex so that $\overline{W_1W_2} \subset \{xY.k\}$. Then also $\overline{W_1W_2} \subset \{xY\}$ which was to be proved in theorem 3. As far as theorem 2 is concerned it is sufficient to realize that $\overline{W_1W_2}$ is a path connecting the Niggli points of L_1, L_2.

(ii) Let the Niggli points W_1, W_2 of L_1, L_2 be connected by a path $\mathbf{P}$ (which may be, in particular, the straight segment $\overline{W_1W_2}$) such that all points of $\mathbf{P}$ are Niggli points of lattices of the same Bravais type, say xY. The $\mathbf{P} \subset \{xY\}$ and W_1, $W_2 \in \{xY\}$. In particular,

$$W_1 \in \{xY.k\}, \qquad W_2 \in \{xY.l\}$$

for some integers k, l. Any of the sets

$$\{xY.k\}, \qquad \mathbf{P}, \qquad \{xY.l\}$$

is connected. The first two have a common point as well as the last two. Thus the union

$$\{xY.k\} \cup \mathbf{P} \cup \{xY.l\}$$

is connected and is a part of $\{xY\}$. Therefore it must be a part of a component $\mathbf{C}$ of $\{xY\}$. Then also

$$\{xY.k\} \subset \mathbf{C}, \qquad \{xY.l\} \subset \mathbf{C}.$$

But $\{xY.k\}$, $\{xY.l\}$ are components of $\{xY\}$ themselves. This is possible only if

$$\{xY.k\} = \mathbf{C} = \{xY.l\}$$

and this means that L_1, L_2 are of the same Niggli character.

Definitions

The necessary and sufficient conditions in theorems 1, 2, 3 enable one to formulate three equivalent definitions of the Niggli characters. The geometrical form of theorems 2 and 3 is replaced by a 'dynamical' version which may be, perhaps, preferred by the physicists.

Definition 1. Let L_1, L_2 be arbitrary lattices of the same Bravais type, say xY. We say that they are of the same Niggli character if their Niggli points belong to the same component of the set $\{xY\}$.

Definition 2 (de Wolff, 1983).* Let L_1, L_2 be arbitrary lattices. We say that they are of the same Niggli character if one of them can be deformed into the other in such a way that the Niggli point of the deformed lattice moves continuously from the initial to the final position while the Bravais type of the lattice remains unchanged.

Definition 3. In definition 2 replace the single word continuously by the word linearly.

Remark 2. The continuous motion of the Niggli point in definition 2 means a continuous deformation of the lattice.† On the other hand, not every continuous deformation of a lattice results in a continuous motion of its Niggli point. The Niggli cell namely can – as a mere abstract notion – 'jump' discontinuously from one cell of the lattice to another. Thus, the continuous deformation of a lattice is a more general condition than the continuous change of the parameters of the Niggli cell. This condition may be used for defining new 'characters' (Wondratschek, 1986) which are more general than the Niggli characters and, moreover, do not depend on the (more or less *ad hoc*) choice of the Niggli cell. This concept, however, has not been studied in this paper.

Remark 3. The linear movement of the Niggli point in definition 3 need not mean a linear change of the parameters a, b, c of the Niggli cell.

* To get a strict equivalence between definition 2 and de Wolff's alternative definition (de Wolff, 1983, 1988) we have to add in definition 2 the assumption that the parameter C changes continuously during the deformation.

† If also the parameter C changes continuously.

Remark 4. All definitions justify the cell-type criterion emphasized by de Wolff (1988).

Remark 5. The Niggli cell, though generally used, is not the only reduced cell which can characterize the lattice in a unique way. At least four such cells can be introduced in a sensible way (Gruber, 1989). The Niggli cell is only one of them and does not differ in principle from the others. This means a serious limitation in the generality of the Niggli characters. We cannot consider them as such a fundamental concept as, for example, the Bravais types. On the other hand, the method worked up in this paper for the Niggli cells can be applied also to other reduced cells. Only the Niggli points will be replaced by another kind of representative point (*e.g.* those which belong to the cells fulfilling $a+b+c=$ abs min, surface = rel min). Instead of the sets $\{xY\}$ we shall now get some other sets which may be denoted, say, $[xY]$. Then definition 1 in a proper modification will create new kinds of 'characters'. Whether also definitions 2 and 3 will have their analogies depends on the shape of the sets $[xY]$. The details, however, are not investigated here.

Concluding remarks

Any of the three definitions 1, 2, 3 is equivalent to the hitherto used procedure based on the Niggli table and determines the same classes of lattices of the same Niggli character.* In this way, perhaps, the Niggli characters are defined as clearly as the Bravais types and systems.

The author thanks Professor P. M. de Wolff (Delft) for many years of correspondence on Niggli characters and Professor H. Wondratschek (Karlsruhe) for inspiring discussions. His thanks are also due to a referee for calling his attention to some papers on this subject.

APPENDIX

The Niggli table

The Niggli table is presented here in a modification for the 'reduced' parameters (Table 3). The given data [*i.e.* the normalized 'reduced' parameters (4) of the lattice] are compared with the entries in the order in which the entries appear in the table. The blank spaces are ignored (*i.e.* from the parameter in question nothing is required). The first agreement determines the Nigglie character. For example, the lattice with $(u, v, x, y, z) = (\frac{1}{2}, \frac{1}{2}, \frac{1}{8}, \frac{1}{4}, \frac{1}{2})$ is of the Niggli character *mC*.29.

* The conventional notation of the particular characters must be, of course, added.

Table 3. *Niggli table*

(*a*) For the positive Niggli characters

u	v	x	y	z	Character
1	1	1	1	1	*cF*.1
1	1		x	x	*hR*.2
	u	u	u	u	*hR*.9
	u		x		*mC*.10
$2x$	1		u	u	*tI*.18
	1		u	u	*oI*.19
	1			y	*mC*.20
$2x$			u	u	*oF*.26
			u	u	*mC*.27
			u	$2x$	*mC*.28
			$2x$	u	*mC*.29
		v		$2y$	*mC*.30
					aP.31

(*b*) For the non-positive Niggli characters
Notation: $s=u+v+x+y+z$, $w=2u+2y+z$

u	v	x	y	z	s	w	Character
1	1	0	0	0			*cP*.3
1	1		x	x	0		*cI*.5
1	1		x	x			*hR*.4
1	1		x		0		*tI*.6
1	1			y	0		*tI*.7
1	1				0		*oI*.8
	u	0	0	0			*tP*.11
	u	0	0	$-u$			*hP*.12
	u	0	0				*oC*.13
	u	$-u$	$-u$	0			*tI*.15
	u		x		0		*oF*.16
	u		x				*mC*.14
	u				0		*mC*.17
	1	0	0	0			*tP*.21
	1	-1	0	0			*hP*.22
	1		0	0			*oC*.23
	1			y	0	0	*hR*.24
	1			y			*mC*.25
		0	0	0			*oP*.32
		$-v$	0	0			*oC*.40
			0	0			*mP*.35
		0	$-u$	0			*oC*.36
		0		0			*mP*.33
		0	0	$-u$			*oC*.38
		0	0				*mP*.34
		$-v$	$-u$	0			*oI*.42
		$-v$		0			*mC*.41
			$-u$	0			*mC*.37
			0	$-u$			*mC*.39
					0	0	*mC*.43
							aP.44

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A Class of Patterns Generated by Modification of Beenker's Pattern

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Abstract

A modification of Beenker's pattern is considered that is generated by the transformation matrix obtained by applying the rotation matrix to that for Beenker's pattern. The symmetry of the modified pattern is discussed based on the transformation matrix. It is well known that Beenker's pattern, a two-dimensional eightfold quasiperiodic pattern, is characterized by the transformation matrix, the column vectors of which are the projected basis vectors in four-dimensional cubic lattice space.

1. Introduction

The theory of quasiperiodic patterns has been extensively studied in connection with the modeling of quasicrystals (Bak & Goldman, 1988). Among many methods of generating quasiperiodic patterns, the projection method is a standard and widely used method (Bak & Goldman, 1988). In this paper a two-dimensional eightfold symmetric quasiperiodic pattern or tiling called Beenker's pattern is reviewed first. It is generated by the projection method from the four-dimensional cubic lattice to the two-dimensional pattern space so as to have eightfold symmetry. Then, the modification of this pattern is considered by introducing an orthogonal transformation matrix based on the rotation in four-dimensional space. The rotation of the transformation matrix defining the pattern and test spaces (see § 2) has been considered by Kramer (1987) in connection with icosahedral and cubic symmetries. The phason strain, another kind of modification or deformation, with respect to Beenker's pattern is treated by Wang & Kuo (1988) and Socolar (1989).

2. A two-dimensional eightfold symmetric quasiperiodic pattern

It is known that a two-dimensional eightfold symmetric quasiperiodic pattern, Beenker's pattern (Beenker, 1982) is characterized by the orthogonal transformation matrix A (Wang & Kuo, 1988; Socolar, 1989; Soma, Watanabe & Ito, 1990),

$$A = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1/\sqrt{2} & 0 & -1/\sqrt{2} \\ 0 & 1/\sqrt{2} & 1 & 1/\sqrt{2} \\ 1 & -1/\sqrt{2} & 0 & 1/\sqrt{2} \\ 0 & 1/\sqrt{2} & -1 & 1/\sqrt{2} \end{pmatrix}. \tag{1}$$

The column vectors correspond to basis vectors of the original axes (x_i) with respect to the transformed axes (x'_j). Since the upper and the lower two rows correspond to the pattern (parallel) and the test (perpendicular) space, respectively (Soma, Watanabe & Ito, 1990), the upper and lower two-dimensional column vectors $\mathbf{a}_i^{\parallel}$ and $\mathbf{a}_j^{\perp}$ ($i, j = 1, 2, 3, 4$) represent the projected basis vectors in their respective spaces as shown in Fig. 1. It is known that the pattern consists of a square and a rhombus of equal-length sides, as shown in Fig. 2. The pattern is thought of as a mixture of two square lattices rotated relative to each other by $\pi/4$. It is easy to see that the matrix A is generated by the product of four simple rotation matrices in four-dimensional space,

$$A = R_{13}(\alpha_{13})R_{24}(\alpha_{24})R_{34}(\alpha_{34})R_{23}(\alpha_{23}), \tag{2}$$

with $\alpha_{13} = -\pi/4$, $\alpha_{24} = \pi/4$, $\alpha_{34} = \pi/4$ and $\alpha_{23} = \pi/2$, where $R_{ij}(\alpha_{ij})$ is the matrix representing a simple rotation in the $x_i x_j$ plane by an angle α_{ij} from the axis x_i toward the x_j axis, such as

$$R_{12}(\alpha_{12}) = \begin{pmatrix} \cos\alpha_{12} & \sin\alpha_{12} & 0 & 0 \\ -\sin\alpha_{12} & \cos\alpha_{12} & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \tag{3}$$

As is discussed by Wang & Kuo (1988), the pattern generated by the transformation matrix A has sym-

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