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Aperiodic Tilings with Non-Symmorphic Space Groups $p2^jgm$

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Abstract

As an illustrative application of the general theory of quasicrystallographic space groups a non-symmorphic aperiodic tiling is constructed with space group $p2^jgm$ using a generalization of the grid method.

I. Introduction

The discovery of alloys called 'quasicrystals' (Schechtman, Blech, Gratias & Cahn, 1984; Levine & Steinhardt, 1984) with diffraction patterns containing sharp Bragg-like peaks with non-crystallographic point-group symmetries has stimulated a reexamination of the basic crystallographic concepts of lattice and space group.

If the lattice is defined in Fourier space to be the smallest set of wave vectors $\mathbf{k}$, closed under addition and subtraction, that contains all wave vectors in the diffraction pattern, then there is no reason to require a minimum separation between lattice vectors. Since the proof that lattice point groups can only have two-, three-, four- or sixfold axes requires a minimum separation, such lattices can have arbitrary point-group symmetries. Of course a lattice with a non-crystallographic point group will not be dual to a lattice of translations describing the real-space translational symmetry of the material producing the diffraction pattern. Such materials have lattices only in Fourier space, unless one chooses to view them as real-space projections of higher-dimensional periodic structures.

Materials characterized by a Fourier space lattice with point-group symmetry G can be further classified by the phase relations between density Fourier coefficients $\rho(\mathbf{k})$ at symmetry-related points. These relations fall into certain equivalence classes, described more fully below, which in the crystallographic case correspond precisely to the ordinary space groups, and which define the concept of a space group in the non-crystallographic case.

Such an analysis of the two-dimensional quasicrystallographic space groups has been given by Rokhsar, Wright & Mermin (RWM) (1988) for 'standard lattices'. The standard two-dimensional lattice with N-fold rotational symmetry is the set of all integral linear combinations of N wave vectors of equal length separated by angles of $2\pi/N$. Mermin, Rokhsar & Wright (1987) have shown that all two-dimensional lattices are standard when $N<46$, but for larger N non-standard lattices abound. (Although there is only one class of 4-, 8-, 16-, and 32-lattices, there are, for example, 17 distinct 64-lattices and 359 057 distinct 128-lattices, where 'distinct' means differing by more than just a rotation and/or rescaling.)

The two-dimensional space groups belonging to standard lattices with N-fold symmetry are very simple when N is not a power of 2: all phase relations belong to the same class as the trivial one that assigns identical phases to Fourier coefficients at symmetry-related points. In the crystallographic case such space groups are called 'symmorphic', and it is natural to extend this nomenclature to the non-crystallographic case.

When N is a power of 2, however, the standard lattice can also have a non-symmorphic space group, characterized by non-trivial phase relations, which require systematic extinctions – the vanishing of Fourier coefficients at certain wave vectors. When the point group is 2^jmm, RWM call the symmorphic and non-symmorphic quasicrystallographic space groups $p2^jmm$ and $p2^jgm$. This reduces to the standard crystallographic notation when $j=2$.

In their paper RWM display patterns with $p8mm$ and $p8gm$ symmetry, constructed by taking linear combinations of a small number of plane waves with the appropriate phase relations. In constructing models of real materials, however, one exploits examples of the space groups that consist of sets of real-space points with a minimum distance between them. This is commonly done by taking the points to be the vertices of an aperiodic tiling of the appropriate

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point-group symmetry or, often equivalently, to be the projection into physical space of a slice of a higher-dimensional periodic array.

Such methods for constructing tilings with $p2^jmm$ symmetry are well known, and many examples can be found in the literature (*e.g.* de Bruijn, 1981; Duneau & Katz, 1985; Gähler & Rhyner, 1986; Elser, 1986). We describe here a method for constructing tilings with the non-symmorphic $p2^jgm$ space-group symmetry. The fruits of this procedure are displayed in Fig. 1, which shows tilings with the symmorphic space group $p8mm$ and the non-symmorphic space group $p8gm$. For comparison Fig. 2 shows the periodic $p4mm$ and $p4gm$ tilings that result when the same procedure is applied to the crystallographic case. Readers content with perusing pictures are invited to enjoy Fig. 1(*b*), hunt for evidence of 'quasi-glide lines', and turn to more pressing matters. For readers interested in the process of construction, the rest of the paper is organized as follows: In § II we describe the new algorithm that gives the $p2^jgm$ tilings (together with the familiar algorithm giving the symmorphic $p2^jmm$ tilings). In § III we summarize the definitions and results of RWM that we need to specify the conditions for a tiling to have the non-symmorphic space group $p2^jgm$. In § IV we give a simple formulation of the relation between tilings and projections from higher dimensions, which some readers might find of interest in itself. In § V we apply the formulation of § IV to a proof that the Fourier coefficients of a sum of δ functions at the vertices of the tilings described in § II do indeed have the phase relations described in § III.

II. Tilings with $p2^jgm$ symmetry

First we describe the conventional grid method (de Bruijn, 1981; Socolar, Steinhardt & Levine, 1985; Gähler & Rhyner, 1986) for constructing a tiling with 2^j-fold symmetry and the symmorphic space group $p2^jmm$. Then we describe a simple modification of that construction that yields a non-symmorphic tiling with $p2^jgm$ symmetry. These space-group identifications are made in § V.

A. The symmorphic tiling

Consider an infinite family of parallel lines separated by a distance L and normal to the direction $\mathbf{n}$ (Fig. 3). Next, consider the grid given by superimposing $D = N/2$ such families (in the case of interest for us N is a power of 2), all with the same wavelength L, whose normals are separated by angles $2\pi/N$ (Fig. 4). For appropriate choice of phase in each family (for example if all families contain a line passing through the origin, or if the origin lies midway between two adjacent lines of each family) the resulting grid will have 2^jmm symmetry. However, as will be demonstrated in § IV, the constructions to be described produce tilings with the desired space groups for any choice of these phases.

A tiling is constructed from the grid as follows: pick an arbitrary polygonal cell in the grid and an arbitrary point in a second plane, the tiling plane, which we shall say *corresponds* to the cell in the grid. Then wander about in the grid. Each time you cross a boundary to a new cell, draw a line in the tiling plane of length a along the direction of the outward normal from the old cell to the new one. That line connects the point corresponding to the old cell to the point that will correspond to the new cell (Fig. 5). It is easy to show that the structure you end up with, after every side shared by every pair of neighboring cells has been crossed at least once, does not depend on how you wander through the grid.* This will also be evident from the formalization of this intuitive procedure described in § IV, which we use in § V to show that this construction produces the symmorphic tiling $p2^jmm$.

B. The non-symmorphic tiling

A very simple modification in the above procedure produces a tiling with the space group $p2^jgm$. First label alternate lines in each family 'odd' or 'even'. Then proceed as before, except that after taking a step of length a in the tiling plane along the outward normal when crossing the boundary between two cells, take a second step of an unrelated length c at 90° to the first.† The second step is to the right or left of the first, depending on whether the boundary just crossed is a segment of an odd or even labeled line. Thus the full steps associated with the lines in each family are no longer normal to the lines but alternate from one side of the normal to the other (Fig. 6).

More formal descriptions of these constructions will be given in §§ IV and V, together with proofs that they have the space-group symmetries claimed for them, but first we must specify more precisely what is meant by a quasicrystallographic space group.

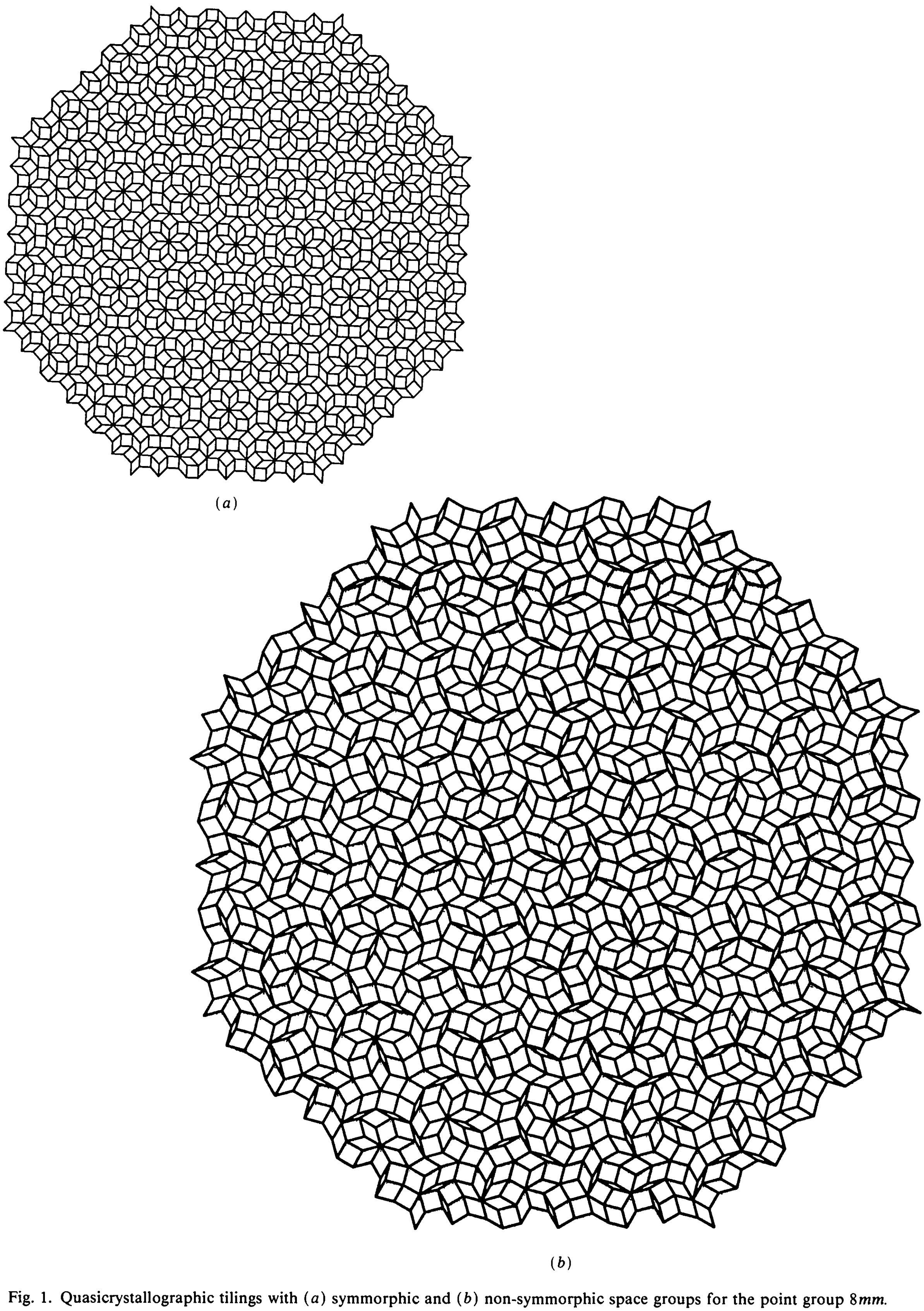
III. Quasicrystallographic space groups

In this section we summarize the definitions and results of RWM relevant to the construction of tilings with $p2^jgm$ symmetry. We are interested in densities of the form

$$\rho(\mathbf{r}) = \sum \rho(\mathbf{k}) \exp(i\mathbf{k}\,.\,\mathbf{r}), \tag{3.1}$$

* The resulting tiles are associated with vertices of the grid and are rhombi except for those vanishingly few vertices at which more than two lines happen to meet.

† By 'unrelated' we mean that the sum of the two steps for one family must not coincide with the sum of the two steps for any other family, so that none of the resulting vertices coincide.



(*a*)

(*b*)

Fig. 1. Quasicrystallographic tilings with (*a*) symmorphic and (*b*) non-symmorphic space groups for the point group $8mm$.

where the sum is over all wave vectors in the lattice generated by n vectors $\mathbf{v}^{(j)}$ that are linearly independent over the integers,

$$\mathbf{k}=\sum_{j=1}^{n} n_j \mathbf{v}^{(j)}. \tag{3.2}$$

(For plane lattices with 2^j-fold symmetry one requires 2^{j-1} such generating vectors.)

The point group G of a material is the symmetry group of all its macroscopic translationally invariant equilibrium properties. In particular the diffraction pattern, and hence the lattice of wave vectors it gives rise to, is invariant under G, as is the product of any group of Fourier coefficients the sum of whose wave vectors vanishes:

$$\rho(\mathbf{k})\rho(\mathbf{k}')\rho(\mathbf{k}'')\ldots=\rho(g\mathbf{k})\rho(g\mathbf{k}')\rho(g\mathbf{k}'')\ldots$$
$$\text{whenever}\quad \mathbf{k}+\mathbf{k}'+\mathbf{k}''+\ldots=0, \tag{3.3}$$

for all operations g in G.

Equation (3.3) requires the Fourier coefficients at symmetry-related points to be related by

$$\rho(g\mathbf{k})=\exp\left[2\pi i\Phi_g(\mathbf{k})\right]\rho(\mathbf{k}), \tag{3.4}$$

where for each g the 'phase function' $\Phi_g(\mathbf{k})$ must satisfy

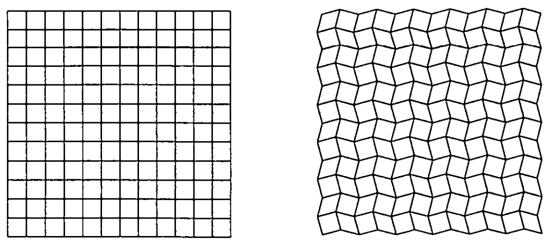
$$\Phi_g(\mathbf{k})+\Phi_g(\mathbf{k}')+\Phi_g(\mathbf{k}'')+\ldots\equiv 0$$
$$\text{whenever}\quad \mathbf{k}+\mathbf{k}'+\mathbf{k}''+\ldots=0, \tag{3.5}$$

where $\equiv$ denotes equality to within an integer.

Because of the linearity condition (3.5) it is enough to specify the phase functions for the generating vectors $\mathbf{v}^{(j)}$, $j=1,\ldots,n$. Furthermore, because $\rho[(gh)\mathbf{k}]=\rho[g(h\mathbf{k})]$, the phase functions Φ_g for all elements g of the group G must satisfy

$$\Phi_{gh}(\mathbf{k})=\Phi_g(h\mathbf{k})+\Phi_h(\mathbf{k}). \tag{3.6}$$

As a result of this relation all the phase functions can be determined from those for any subset of the elements that generates the entire group. In the case of two-dimensional point groups it therefore suffices to determine the phase function Φ_r for a rotation r through $2\pi/N$, and (if the group possesses



(a) $p4mm$ (b) $p4gm$

Fig. 2. The analogous crystallographic tilings with (a) symmorphic and (b) non-symmorphic space groups for the point group $4mm$.

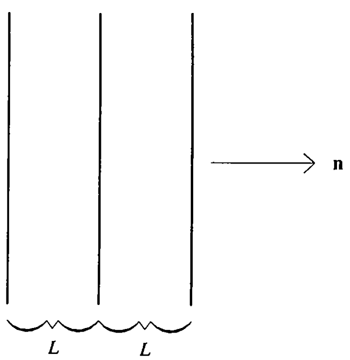


Fig. 3. Three lines from an infinite family with wavelength L and normal $\mathbf{n}$.

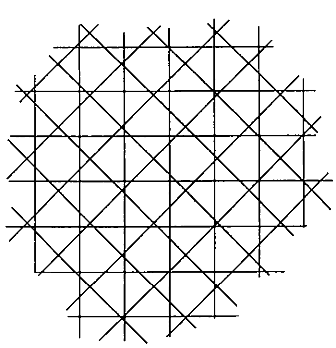


Fig. 4. Part of an $N=8$ grid with randomly chosen phases.

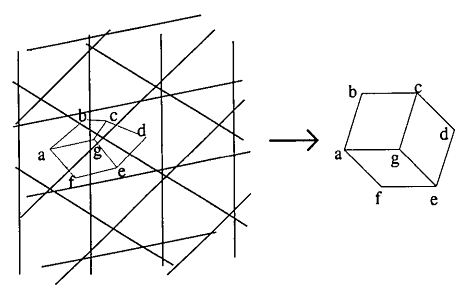


Fig. 5. The grid on the left produces the tiling on the right by mapping cells (labeled by letters) to corresponding vertices and vertices to rhombi as described in § II.A.

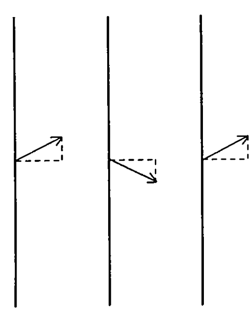


Fig. 6. The tiling vectors $\mathbf{a}\pm\mathbf{c}$ for the non-symmorphic construction described in §II.B.

mirrorings) the phase function Φ_m for any one mirror element.

The possible phase functions fall naturally into classes of mutually equivalent functions. This is because two densities related by

$$\rho'(\mathbf{k}) = \exp[2\pi i\chi(\mathbf{k})]\rho(\mathbf{k}) \tag{3.7}$$

give the same value for all quantities of the form (3.3) and are therefore macroscopically indistinguishable, if and only if the difference in phase satisfies the condition

$$\chi(\mathbf{k}) + \chi(\mathbf{k}') + \chi(\mathbf{k}'') + \ldots \equiv 0$$
$$\text{whenever} \quad \mathbf{k} + \mathbf{k}' + \mathbf{k}'' + \ldots = 0. \tag{3.8}$$

Such a linear function is called a 'gauge function'.

If two densities differ in phase only by such a gauge function (in the terminolgy of quasicrystals they then differ only by a real-space translation and a phason) then the corresponding sets of phase functions are said to be equivalent. Equivalent sets of phase functions are thus related by a 'gauge transformation' of the form

$$\Phi'_g(\mathbf{k}) - \Phi_g(\mathbf{k}) \equiv \chi(g\mathbf{k}) - \chi(\mathbf{k}), \tag{3.9}$$

where the gauge function χ is independent of the group element g. For the tilings to be discussed here, distinct space groups correspond to distinct classes of phase functions.*

For two-dimensional standard lattices RWM show that all phase functions are equivalent to a set of identically zero phase functions (and therefore all space groups are symmorphic) except when the point group is 2^jmm. In that one case, there can be two distinct space groups: the symmorphic space group $p2^jmm$, with all phase functions equivalent to zero, and the non-symmorphic space group $p2^jgm$, for which the phase function Φ_r can still be taken to be zero with a suitable choice of gauge, but for which there is no gauge in which the phase function Φ_m vanishes. The hallmark of the non-symmorphic space group is that if m_j is the mirroring that leaves the generating vector $\mathbf{v}^{(j)}$ invariant, then $\Phi_{m_j}(\mathbf{v}^{(j)})$ [which (3.9) requires to be gauge invariant] satisfies

$$\Phi_{m_j}(\mathbf{v}^{(j)}) \equiv \tfrac{1}{2}. \tag{3.10}$$

In conjunction with (3.4) this leads to extinctions: $\rho(\mathbf{k})$ must vanish for wave vectors that are odd multiples of any given generating vectors $\mathbf{v}^{(j)}$.

IV. Tilings and projections: some useful relations

We now describe a way to characterize a very general class of tilings in terms of projections from higher-dimensional spaces. We shall use this approach in § V to establish that the tilings described in § II do indeed have the space-group symmetries claimed for them. This way of relating tilings and projections is in some respects simpler than those to be found in the literature, so we describe it here in a more general setting than we shall actually need for the application in § V.

A. Grid wave vectors and tiling vectors

We are given an arbitrary set of 'grid wave vectors',

$$\mathbf{k}^{(j)} = 2\pi\mathbf{n}^{(j)}/L_j, \quad j = 1, \ldots, D, \tag{4.1}$$

which span a 'grid space' of dimension $d < D$. Each wave vector characterizes a family of d-space hyperplanes normal to the direction $\mathbf{n}^{(j)}$ and a distance L_j apart. Each family is also characterized by a fractional displacement

$$f_j = d_j/L_j, \quad j = 1, \ldots, D, \tag{4.2}$$

where d_j (see Fig. 7) is the distance from the origin to the nearest hyperplane of the family in the direction of $-\mathbf{n}^{(j)}$.

Taken together the families of hyperplanes divide the grid space into cells. We assign to each point $\mathbf{R}$ in the interior of any cell an integer n_j which tells where it is with respect to the hyperplanes in the jth family:

$$n_j = [(1/2\pi)\mathbf{k}^{(j)} \cdot \mathbf{R} + f_j], \tag{4.3}$$

where $[x]$ is the largest integer less than x. This rule assigns the number 0 to points between the same pair of hyperplanes as the origin and simply increases the number n_j by 1 as each hyperplane in the family is crossed in the direction of its normal $\mathbf{n}^{(j)}$ (de Bruijn, 1981; Gähler & Rhyner, 1986).

We are also given a set of tiling vectors $\mathbf{a}^{(j)}$, $j = 1, \ldots, D$, which span a d-dimensional tiling space. The vertices of the tiling consist of all points of the form

$$\sum_{j=1}^{D} n_j \mathbf{a}^{(j)} \tag{4.4}$$

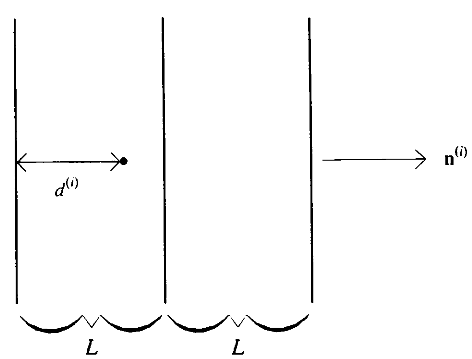


Fig. 7. The family of Fig. 3 displaced a distance $d^{(i)}$ from the origin (marked with a solid circle).

* For our purposes the term 'space group' simply means 'equivalence class of phase functions'. The term can, however, be given a group theoretic interpretation. This is discussed in the Appendix.

as $\mathbf{R}$ in (4.3) ranges through all cells of the grid. When the $\mathbf{a}^{(j)}$ are arbitrary and entirely unrelated to the $\mathbf{k}^{(j)}$ we have the case discussed by Gähler & Rhyner (1986). Our intuitive description of the $p2^jmm$ tiling in § II is equivalent to this more formal description if the families of hyperplanes are taken to be the 2^{j-1} symmetric families of lines in the plane, and the tiling vectors are simply the normals to the families:

$$\mathbf{a}^{(j)}=a\mathbf{n}^{(j)}. \tag{4.5}$$

In this section, we shall consider more generally any sets of tiling vectors $\mathbf{a}^{(j)}$ and grid wave vectors $\mathbf{k}^{(j)}$ that are related by the condition*

$$\sum_{j=1}^{D} a_\mu^{(j)}k_\nu^{(j)}=2\pi\delta_{\mu\nu}. \tag{4.6}$$

The $p2^jmm$ tiling of § II satisfies condition (4.6) if we pick the length a to be $2L/D$.

B. Extension to D dimensions

Given any set of tiling vectors $\mathbf{a}^{(j)}$ that satisfy (4.6) with a set of grid vectors $\mathbf{k}^{(j)}$, we can extend the two sets of vectors to mutually orthogonal sets in D dimensions. For it follows from (4.6) that if

$$\sum_{\mu=1}^{d} c_\mu a_\mu^{(j)}=0,\quad j=1,\ldots,D, \tag{4.7}$$

then all the coefficients c_μ must vanish. This establishes that if

$$a_1^{(j)},\ldots,a_d^{(j)} \tag{4.8}$$

are considered as a set of d vectors in D dimensions with components indexed by $j=1,\ldots,D$, then they are linearly independent. The same argument can be made for the set

$$k_1^{(j)},\ldots,k_d^{(j)}. \tag{4.9}$$

Now let the $D-d$ vectors

$$q_{d+1}^{(j)},\ldots,q_D^{(j)} \tag{4.10}$$

span the $(D-d)$-dimensional subspace of D-space orthogonal to the d-dimensional subspace spanned by the set (4.8), so that we have

$$\sum_{j=1}^{D} a_\mu^{(j)}q_\nu^{(j)}=0. \tag{4.11}$$

Note that in D dimensions the d vectors $k_\mu^{(j)}$ and the $D-d$ vectors $q_\mu^{(j)}$ constitute a linearly independent set, for if

$$\sum_{\mu=1}^{d} e_\mu k_\mu^{(j)}+\sum_{\mu=d+1}^{D} f_\mu q_\mu^{(j)} \tag{4.12}$$

vanishes for all j, then by multiplying (4.12) by $a_\nu^{(j)}$, summing on j, and appealing to (4.6) and (4.11), one establishes that the e_ν all vanish. The vanishing of the f_ν as well then follows from the linear independence of the $q_\mu^{(j)}$ in their $(D-d)$-dimensional subspace.

It follows from this independence that the $D\times D$ matrix whose jth row is given by

$$k_1^{(j)},\ldots,k_d^{(j)},\ q_{d+1}^{(j)},\ldots,q_D^{(j)} \tag{4.13}$$

has an inverse; *i.e.* there are quantities $c_\mu^{(i)}$ and $b_\mu^{(i)}$ satisfying

$$\sum_{\mu=1}^{d} c_\mu^{(i)}k_\mu^{(j)}+\sum_{\mu=d+1}^{D} b_\mu^{(i)}q_\mu^{(j)}=2\pi\delta_{ij}. \tag{4.14}$$

Multiplying both sides of (4.14) by $a_\lambda^{(j)}$, summing on j, and appealing to (4.6) and (4.11), one establishes that

$$c_\lambda^{(j)}=a_\lambda^{(j)}. \tag{4.15}$$

It follows from (4.14) and (4.15) that given any two sets of D d-dimensional vectors $\mathbf{a}^{(j)}$ and $\mathbf{k}^{(j)}$ satisfying (4.6), there are two additional sets of D vectors $\mathbf{b}^{(j)}$ and $\mathbf{q}^{(j)}$ of dimension $D-d$, such that the two sets of D-vectors $\mathbf{A}^{(j)}=(\mathbf{a}^{(j)},\mathbf{b}^{(j)})$ and $\mathbf{K}^{(j)}=(\mathbf{k}^{(j)},\mathbf{q}^{(j)})$ constitute mutually orthogonal D-dimensional sets:

$$\mathbf{A}^{(i)}\cdot\mathbf{K}^{(j)}=\mathbf{a}^{(i)}\cdot\mathbf{k}^{(j)}+\mathbf{b}^{(i)}\cdot\mathbf{q}^{(j)}=2\pi\delta_{ij}. \tag{4.16}$$

An important consequence of the D-dimensional orthonormality condition (4.16) is the D-dimensional completeness relation,

$$\sum_{j=1}^{D} A_\mu^{(j)}K_\nu^{(j)}=2\pi\delta_{\mu\nu}, \tag{4.17}$$

which contains (4.6) and also gives

$$\sum_{j=1}^{D} b_\mu^{(j)}q_\nu^{(j)}=2\pi\delta_{\mu\nu}, \tag{4.18}$$

$$\sum_{j=1}^{D} a_\mu^{(j)}q_\nu^{(j)}=0, \tag{4.19}$$

$$\sum_{j=1}^{D} b_\mu^{(j)}k_\nu^{(j)}=0. \tag{4.20}$$

C. Existence of tiling vectors for any set of grid vectors

We note, in passing, that given any set of D grid wave vectors $\mathbf{k}^{(j)}$, one can always find a (not necessarily unique) set of D tiling vectors $\mathbf{a}^{(j)}$ that satisfy (4.6). To do this note first that because the $\mathbf{k}^{(j)}$ span the d-dimensional space, no non-zero d-vector

* The advantages of imposing the condition (4.6) on the otherwise general grid and tiling vectors considered by Gähler & Rhyner (1986) are the simplicity of the ensuing analysis and the absence of any need for a final linear transformation in the tiling plane to establish the connection between tilings and projections. We show in subsection C below that, given any set of grid vectors (4.1), there are always sets of tiling vectors that satisfy (4.6).

can be orthogonal to all of them: if

$$\sum_{\mu=1}^{d} c_\mu k_\mu^{(j)} = 0, \quad j = 1, \ldots, D, \qquad (4.21)$$

then all the coefficients c_μ must vanish. If we again view the

$$k_1^{(j)}, \ldots, k_d^{(j)}, \quad j = 1, \ldots, D \qquad (4.22)$$

as a set of d vectors in D dimensions, then this establishes their linear independence. One can therefore choose $D-d$ additional D-vectors,

$$q_{d+1}^{(j)}, \ldots, q_D^{(j)}, \quad j = 1, \ldots, D, \qquad (4.23)$$

such that the set

$$\mathbf{K}^{(j)} = (\mathbf{k}^{(j)}, \mathbf{q}^{(j)}), \quad j = 1, \ldots, D, \qquad (4.24)$$

spans the entire D-dimensional space. One can next construct a dual basis $\mathbf{A}^{(j)}$, $j = 1, \ldots, D$ for the D-space, that satisfies the orthonormality condition (4.16). If one expands the $\mathbf{A}^{(j)}$ into components in the d- and $(D-d)$-dimensional subspaces as the $\mathbf{K}^{(j)}$ are expanded in (4.24),

$$\mathbf{A}^{(j)} = (\mathbf{a}^{(j)}, \mathbf{b}^{(j)}), \quad j = 1, \ldots, D, \qquad (4.25)$$

then the completeness relation (4.17) gives the required relation (4.6) when μ and ν are restricted to the first d components.

D. Tilings and projections

Suppose now that we have a set of integers of the form (4.3); *i.e.* there is a vector $\mathbf{R}$ such that, for $j = 1, \ldots, D$,

$$n_j = (1/2\pi)\mathbf{k}^{(j)} . \mathbf{R} + f_i - \lambda_j, \quad 0 < \lambda_j < 1. \quad (4.26)$$

If we multiply (4.26) by the $(D-d)$-vector $\mathbf{b}^{(j)}$, sum on j, and use the completeness relation (4.20), we find that

$$\sum_{j=1}^{D} (n_j - f_j)\mathbf{b}^{(j)} = -\sum_{j=1}^{D} \lambda_j \mathbf{b}^{(j)}, \quad 0 < \lambda_j < 1. \quad (4.27)$$

Conversely, suppose we have a set of integers n_j for which (4.27) holds. If we define

$$\mathbf{R} = \sum_{j=1}^{D} (n_j + \lambda_j - f_j)\mathbf{a}^{(j)}, \qquad (4.28)$$

it then follows from (4.27) and the orthonormality condition (4.16) that the n_j do indeed satisfy (4.26).

Consequently a point $\sum n_j \mathbf{a}^{(j)}$ will be a vertex of the tiling if and only if the $(D-d)$-vector $\sum (n_j - f_j)\mathbf{b}^{(j)}$ lies in the convex set

$$-\sum_{j=1}^{D} \lambda_j \mathbf{b}^{(j)}, \quad 0 < \lambda_j < 1. \qquad (4.29)$$

This analytic result can be given a geometrical interpretation by noting that the points of the general D-dimensional lattice primitively generated by the D-vectors $(\mathbf{a}^{(j)}, \mathbf{b}^{(j)})$, $j = 1, \ldots, D$, are points of the form

$$\sum_{j=1}^{D} n_j(\mathbf{a}^{(j)}, \mathbf{b}^{(j)}) \qquad (4.30)$$

for all integral n_j. The points $\sum_{j=1}^{D} n_j \mathbf{a}^{(j)}$ of the tiling are simply the projection into the tiling space of those D-dimensional lattice points whose projection $\sum_{j=1}^{D} n_j \mathbf{b}^{(j)}$ into the perpendicular space lies in the intersection of the perpendicular space with the D-dimensional unit parallelepiped

$$\sum_{j=1}^{D} \lambda_j(\mathbf{a}^{(j)}, \mathbf{b}^{(j)}), \quad -1 < \lambda_j < 0, \qquad (4.31)$$

shifted by the vector $\sum f_j \mathbf{b}^{(j)}$.

V. The space groups of the tilings

We now specialize to the case of the two-dimensional grid space with the 2^{j-1} families of lines described in § II.

A. The symmorphic tiling

Suppose we position every family of lines so that the origin of grid space lies midway between a pair of adjacent lines (Fig. 8). The grid will then have $2^j mm$ symmetry about the origin, and the tiling will have $2^j mm$ symmetry about the point in tiling space that corresponds to the cell containing the origin. If the set of vertices of the tiling has $2^j mm$ symmetry, then so must the Fourier coefficients of a sum of δ functions at those vertices, so all phase functions are zero and the space group is $p2^j mm$.

It remains to show that the space group is unaltered by any shifts in the position of the families along the direction of their normals. We do this by showing that such shifts merely alter the Fourier coefficients $\rho(\mathbf{k})$ by a phase that is linear in $\mathbf{k}$ - *i.e.* by a gauge function. In reaching this conclusion we shall, for the first time, *require* the order N of the rotational symmetry to be 2^j.

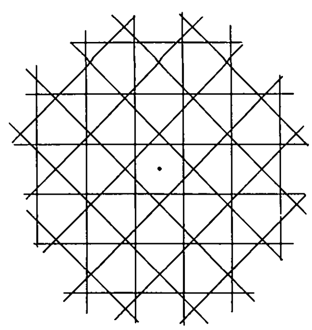


Fig. 8. Part of an $N = 8$ grid with phases chosen to make it symmetric about the origin.

The apparatus developed in § IV applies with the grid vectors taken to be

$$\mathbf{k}^{(j)}=2\pi\mathbf{n}^{(j)}/L,\quad j=1,\ldots,D=N/2,\tag{5.1}$$

where the $\mathbf{n}^{(j)}$ are separated by angles of $2\pi/N$, and the tiling vectors are given by

$$\mathbf{a}^{(j)}=a\mathbf{n}^{(j)}\quad (a=2L/D).\tag{5.2}$$

Let φ be the characteristic function of the set (4.29); *i.e.* $\varphi(\mathbf{s})=1$ or 0 depending on whether or not the $(D-2)$-vector $\mathbf{s}$ is in the set (4.29). Then the sum of two-dimensional δ functions at vertices of the tiling has the form

$$\rho(\mathbf{r})=\sum_{n_1}\ldots\sum_{n_D}\delta\left(\mathbf{r}-\sum_{j=1}^{D}n_j\mathbf{a}^{(j)}\right)\varphi\left(\sum_{j=1}^{D}(n_j-f_j)\mathbf{b}^{(j)}\right),\tag{5.3}$$

where all the n_j are freely summed over.

We can cast this into a simple form by using the representation

$$\sum_{n_1}\ldots\sum_{n_D}\delta\left[(\mathbf{r},\mathbf{s})-\sum_{j=1}^{D}n_j(\mathbf{a}^{(j)},\mathbf{b}^{(j)})\right]$$
$$=\frac{1}{v_D}\sum_{n_1}\ldots\sum_{n_D}\exp\left[i\sum_{j=1}^{D}n_j(\mathbf{k}^{(j)}\cdot\mathbf{r}+\mathbf{q}^{(j)}\cdot\mathbf{s})\right],\tag{5.4}$$

for the sum of D-dimensional δ functions over all points in the D-dimensional lattice that the D independent D-vectors $(\mathbf{a}^{(j)}, \mathbf{b}^{(j)})$ generate primitively. (Here v_D is the volume of the D-dimensional primitive cell of the real-space D-lattice.)

Using this representation, we can equally well write (5.3) as

$$\begin{aligned}\rho(\mathbf{r})=&\int \mathrm{d}\mathbf{s}\,\varphi(\mathbf{s})\\ &\times\sum_{n_1}\ldots\sum_{n_D}\delta\left[(\mathbf{r},\mathbf{s}+\mathbf{f})-\sum_{j=1}^{D}n_j(\mathbf{a}^{(j)},\mathbf{b}^{(j)})\right]\\ =&\frac{1}{v_D}\sum_{n_1}\ldots\sum_{n_D}\exp\left(i\sum_{j=1}^{D}n_j\mathbf{k}^{(j)}\cdot\mathbf{r}\right)\\ &\times\exp\left(i\sum_{j=1}^{D}n_j\mathbf{q}^{(j)}\cdot\mathbf{f}\right)\\ &\times\int \mathrm{d}\mathbf{s}\exp\left(i\sum_{j=1}^{D}n_j\mathbf{q}^{(j)}\cdot\mathbf{s}\right)\varphi(\mathbf{s}),\end{aligned}\tag{5.5}$$

where

$$\mathbf{f}=\sum_{i=1}^{D}f_i\mathbf{b}^{(i)}.\tag{5.6}$$

This explicitly displays the density as a sum of plane waves with wave vectors of the form

$$\mathbf{k}=\sum_{j=1}^{D}n_j\mathbf{k}^{(j)}.\tag{5.7}$$

Because D is a power of 2 (and *only* for such D), the 2-vectors $\mathbf{k}^{(j)}$ for $j=1,\ldots,D$ are integrally independent (see RWM or Hardy & Wright, 1979, pp. 52–53) – *i.e.* the n_j appearing in (5.7) are in fact single-valued functions of the lattice wave vectors and therefore satisfy the linearity condition

$$n_j(\mathbf{k}+\mathbf{k}')=n_j(\mathbf{k})+n_j(\mathbf{k}').\tag{5.8}$$

As a result of this integral independence, any lattice wave vector $\mathbf{k}$ appears in the Fourier expansion (5.5) for only a single term in the sums over $n_1,\ldots,n_D$, and the dependence of the Fourier coefficient $\rho(\mathbf{k})$ on the shifts f_j of the grid lines is entirely through the phase factor $\exp[2\pi i\chi(\mathbf{k})]$, where

$$2\pi\chi(\mathbf{k})=\mathbf{f}\cdot\sum_{j=1}^{D}n_j(\mathbf{k})\mathbf{q}^{(j)}.\tag{5.9}$$

Since the $n_j(\mathbf{k})$ are linear in $\mathbf{k}$ and since $\chi(\mathbf{k})$ is linear in the $n_j(\mathbf{k})$, it follows that $\chi(\mathbf{k})$ is itself linear in $\mathbf{k}$ – *i.e.* it is a gauge function in the sense of § III. This establishes that the space group is indeed independent of the shifts f_j in position of the grids.

B. The non-symmorphic tiling

The vertices of the non-symmorphic tiling described in § II can evidently be described more formally as follows: take each vertex (4.4) that appears in the symmorphic tiling, and give it an additional shift by

$$\sum_{j=1}^{D}p_j\mathbf{c}^{(j)}\tag{5.10}$$

where $\mathbf{c}^{(j)}$ is a displacement of length c at 90° to the right of the displacement $\mathbf{a}^{(j)}$, and p_j is the parity of the integer n_j, being 0 or 1 depending on whether n_j is even or odd.

To investigate the Fourier transform of a sum of δ functions at the resulting set of points, we resolve the entire tiling T into 2^D subtilings, $T_{p_1\ldots p_D}$, associated with the 2^D different parities of the $n_1,\ldots,n_D$. Vertices of the subtiling $T_{p_1\ldots p_D}$ have the form

$$\sum_{j=1}^{D}n_j\mathbf{a}^{(j)}+\sum_{j=1}^{D}p_j\mathbf{c}^{(j)},\tag{5.11}$$

where the integers n_j are those integers (4.26) of the form $n_j=2m_j+p_j$. Thus vertices of the subtiling $T_{p\ldots p_D}$ are the points of the form

$$2\sum_{j=1}^{D}m_j\mathbf{a}^{(j)}+\sum_{j=1}^{D}p_j(\mathbf{a}^{(j)}+\mathbf{c}^{(j)}),\tag{5.12}$$

where the m_j are those integers for which there is a vector $\mathbf{R}$ in grid space satisfying

$$2m_j=(1/2\pi)\mathbf{k}^{(j)}\cdot\mathbf{R}+f_j-p_j-\lambda_j,\quad 0<\lambda_j<1.\tag{5.13}$$

Equations (5.12) and (5.13) reveal that the subtiling $T_{p_1\ldots p_D}$ is obtained from the subtiling $T_{0\ldots0}$ by shifting it in tiling space by $\sum_{j=1}^{D} p_j(\mathbf{a}^{(j)}+\mathbf{c}^{(j)})$ and by shifting each f_i by $-p_i$, *i.e.* shifting $\mathbf{f}$ [(5.6)] by $-\mathbf{p}$, where

$$\mathbf{p}=\sum_{j=1}^{D} p_j\mathbf{b}^{(j)}. \tag{5.14}$$

Now the subtiling $T_{0\ldots0}$, like the symmorphic tiling, can be given 2^jmm symmetry with a suitable choice of the grid displacements f_i. (Arrange for the origin of grid space again to lie at the center of the $0\ldots0$ cell in grid space, and note that $T_{0\ldots0}$ is then just a subset of the similarly symmetrized version of the symmorphic tiling, selected from it by an explicitly symmetric rule.) Consequently, as in the symmorphic case, the Fourier coefficients of $\rho_{0\ldots0}$, the sum of δ functions at the vertices of a $T_{0\ldots0}$ tiling from a grid with general displacements f_i, differ by only a linear gauge function from a set of Fourier coefficients with zero phase functions.

To exploit this fact we first show that the Fourier coefficients of the non-symmorphic tiling $\rho(\mathbf{k})$ are simply proportional to those of $\rho_{0\ldots0}$:

$$\rho(\mathbf{k})=S(\mathbf{k})\rho_{0\ldots0}(\mathbf{k}). \tag{5.15}$$

Since the phase functions of $\rho_{0\ldots0}(\mathbf{k})$ differ from zero only by a gauge function, the phase functions of $\rho(\mathbf{k})$ will differ from those of $S(\mathbf{k})$ only by a gauge transformation [(3.7)]. By explicitly computing $S(\mathbf{k})$ we can therefore determine the space-group symmetry of the non-symmorphic tiling.

First, following the same lines we pursued in the symmorphic case, we express the density of vertices in the subtiling $T_{0\ldots0}$ in a form similar to the expression (5.3) for the symmorphic tiling:

$$\rho_{0\ldots0}(\mathbf{r})=\sum_{m_1}\ldots\sum_{m_D}\delta\left(\mathbf{r}-2\sum_{j=1}^{D} m_j\mathbf{a}^{(j)}\right)\times\varphi\left[\sum_{j=1}^{D}(2m_j-f_j)\mathbf{b}^{(j)}\right]. \tag{5.16}$$

Again using the representation (5.4) of the δ function, we can recast this in the form

$$\begin{aligned}\rho_{0\ldots0}(\mathbf{r})&=\int \mathrm{d}\mathbf{s}\,\varphi(\mathbf{s})\\&\quad\times\sum_{m_1}\ldots\sum_{m_D}\delta\left[(\mathbf{r},\mathbf{s}+\mathbf{f})-2\sum_{j=1}^{D} m_j(\mathbf{a}^{(j)},\mathbf{b}^{(j)})\right]\\&=\frac{1}{2^D}\int \mathrm{d}\mathbf{s}\,\varphi(\mathbf{s})\\&\quad\times\sum_{m_1}\ldots\sum_{m_D}\delta\left[\tfrac{1}{2}(\mathbf{r},\mathbf{s}+\mathbf{f})-\sum_{j=1}^{D} m_j(\mathbf{a}^{(j)},\mathbf{b}^{(j)})\right]\\&=\frac{1}{2^Dv_D}\sum_{n_1}\ldots\sum_{n_D}\exp\left(i\tfrac{1}{2}\sum_{j=1}^{D} n_j\mathbf{k}^{(j)}.\mathbf{r}\right)\\&\quad\times\exp\left(i\tfrac{1}{2}\sum_{j=1}^{D} n_j\mathbf{q}^{(j)}.\mathbf{f}\right)\\&\quad\times\int \mathrm{d}\mathbf{s}\,\varphi(\mathbf{s})\exp\left(i\tfrac{1}{2}\sum_{j=1}^{D} n_j\mathbf{q}^{(j)}.\mathbf{s}\right).\end{aligned} \tag{5.17}$$

Note (in contrast to the symmorphic case) that the wave vectors in the Fourier expansion can now have either integral or half-integral coefficients when expanded in terms of the $\mathbf{k}^{(j)}$. The lattice of wave vectors is therefore generated by the set $\mathbf{v}^{(j)}=\frac{1}{2}\mathbf{k}^{(j)}$, $j=1,\ldots,D$, and any wave vector in the lattice has the expansion

$$\mathbf{k}=\sum_{j=1}^{D} n_j(\mathbf{k})\tfrac{1}{2}\mathbf{k}^{(j)}. \tag{5.18}$$

In view of the simple relation between the subtilings $T_{p_1\ldots p_D}$ and $T_{0\ldots0}$ revealed by (5.12) and (5.13) and (as earlier) in view of the integral independence of $\mathbf{k}^{(1)}\ldots\mathbf{k}^{(D)}$, it follows from (5.17) that the Fourier coefficients $\rho_{p_1\ldots p_D}(\mathbf{k})$ and $\rho_{0\ldots0}(\mathbf{k})$ are related by

$$\rho_{p_1\ldots p_D}(\mathbf{k})=\exp\left[-i\mathbf{k}.\sum_{j=1}^{D} p_j(\mathbf{a}^{(j)}+\mathbf{c}^{(j)})-i\tfrac{1}{2}\mathbf{p}.\sum_{j=1}^{D} n_j(\mathbf{k})\mathbf{q}^{(j)}\right]\rho_{0\ldots0}(\mathbf{k}). \tag{5.19}$$

Using the orthonormality condition (4.16), the definition (5.14) of $\mathbf{p}$, and the expansion (5.18) of $\mathbf{k}$, we can simplify (5.19) to

$$\rho_{p_1\ldots p_D}(\mathbf{k})=(-1)^{\sum_{j=1}^{D} p_jn_j(\mathbf{k})}\times\exp\left(-i\mathbf{k}.\sum_{j=1}^{D} p_j\mathbf{c}^{(j)}\right)\rho_{0\ldots0}(\mathbf{k}). \tag{5.20}$$

Now the density $\rho(\mathbf{k})$ of the entire non-symmorphic tiling is just the sum of the densities of the 2^D subtilings corresponding to all possible choices of 0 or 1 for the D parities p_j. Thus

$$\rho(\mathbf{k})=\prod_{j=1}^{D}\left[1+(-1)^{n_j(\mathbf{k})}\exp(-i\mathbf{k}.\mathbf{c}^{(j)})\right]\rho_{0\ldots0}(\mathbf{k}). \tag{5.21}$$

This establishes (5.15), with the structure factor

$$S(\mathbf{k})=\prod_{j=1}^{D}\left[1+(-1)^{n_j(\mathbf{k})}\exp(-i\mathbf{k}.\mathbf{c}^{(j)})\right]. \tag{5.22}$$

When the additional displacements $\mathbf{c}^{(j)}$ are zero so the tiling reduces back to the symmorphic one, the structure factor vanishes except when all the $n_j(\mathbf{k})$ are even, and the enriched lattice (5.18) indeed reduces back to the lattice of the symmorphic tiling.

Note next that when $\mathbf{k}$ is a multiple of a single generating vector, $\mathbf{k}=n_{j_0}\mathbf{v}^{(j_0)}=\frac{1}{2}n_{j_0}\mathbf{k}^{(j_0)}$, then the term in the product (5.22) with $j=j_0$ vanishes for odd n_{j_0}, since each $\mathbf{c}^{(j)}$ is orthogonal to the corresponding $\mathbf{k}^{(j)}$. The non-symmorphic lattice therefore has precisely the extinctions noted in § III as characteristic of $p2^jgm$ symmetry.

To confirm that the tiling does indeed have point-group symmetry 2^jmm we must show that the phase functions $\Phi_r(\mathbf{k})$ and $\Phi_m(\mathbf{k})$ associated with a rotation r and a mirroring m are indeed linear in $\mathbf{k}$. In addition, to be sure that the extinctions are not accidental extinctions in a structure with space group $p2^jmm$, we must show that the phase function $\Phi_m(\mathbf{k})$ satisfies (3.10).

Let the mirroring m be about $\mathbf{k}_D$. It is evident (Fig. 9) that if $\mathbf{k}_0$ is defined to be $-\mathbf{k}_D$, then

$$m\mathbf{k}^{(j)}=-\mathbf{k}^{(D-j)}, \qquad n_j(m\mathbf{k})=-n_{D-j}(\mathbf{k}),$$
$$j=1,\ldots,D, \tag{5.23}$$

and

$$m\mathbf{k}^{(j)}\,.\,\mathbf{c}^{(i)}=-\mathbf{k}^{(D-j)}\,.\,\mathbf{c}^{(i)}=\mathbf{k}^{(j)}\,.\,\mathbf{c}^{(D-i)}, \tag{5.24}$$

with the conventions

$$\mathbf{c}^{(0)}=-\mathbf{c}^{(D)}, \qquad n_0(\mathbf{k})=-n_D(\mathbf{k}). \tag{5.25}$$

It follows that

$$S(m\mathbf{k})=\prod_{j=1}^{D}\,[1+(-1)^{n_{D-j}(\mathbf{k})}\exp(-i\mathbf{k}\,.\,\mathbf{c}^{(D-j)})]. \tag{5.26}$$

Changing the product index from j to $D-j$, we get back (5.22) with a different set of limits:

$$S(m\mathbf{k})=\prod_{j=0}^{D-1}\,[1+(-1)^{n_j(\mathbf{k})}\exp(-i\mathbf{k}\,.\,\mathbf{c}^{(j)})] \tag{5.27}$$

or

$$S(m\mathbf{k})=\frac{1+(-1)^{n_0(\mathbf{k})}\exp(-i\mathbf{k}\,.\,\mathbf{c}^{(0)})}{1+(-1)^{n_D(\mathbf{k})}\exp(-i\mathbf{k}\,.\,\mathbf{c}^{(D)})}\times\prod_{j=1}^{D}\,[1+(-1)^{n_j(\mathbf{k})}\exp(-i\mathbf{k}\,.\,\mathbf{c}^{(j)})]. \tag{5.28}$$

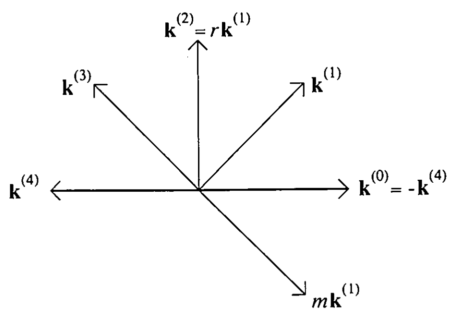


Fig. 9. Mirrorings (m) and rotations (r) of the generating vectors for $D=N/2=4$. Note that $\mathbf{c}^{(j)}$ points perpendicularly and counter-clockwise with respect to $\mathbf{k}^{(j)}$. See equations (5.23) and (5.24).

We conclude [see (5.25)] that

$$S(m\mathbf{k})=(-1)^{n_D(\mathbf{k})}\exp(i\mathbf{k}\,.\,\mathbf{c}^{(D)})S(\mathbf{k}). \tag{5.29}$$

By the definition (3.4) of the phase functions, we also have, to within a gauge transformation, that

$$S(m\mathbf{k})=\exp[2\pi i\Phi_m(\mathbf{k})]S(\mathbf{k}). \tag{5.30}$$

To establish that the vanishing of the structure factor at the extinguished points is not an accident, we must show that $\Phi_m(\frac{1}{2}\mathbf{k}^{(D)})\equiv\frac{1}{2}$. Although $n_D(\frac{1}{2}\mathbf{k}^{(D)})=1$, and $\mathbf{k}^{(D)}\,.\,\mathbf{c}^{(D)}=0$, we cannot infer this immediately from (5.29) and (5.30) because the structure factor S vanishes at $\frac{1}{2}\mathbf{k}^{(D)}$. We can, however, infer that at all points with non-zero structure factors, the phase function is given by

$$\Phi_m(\mathbf{k})=\tfrac{1}{2}n_D(\mathbf{k})+(1/2\pi)\mathbf{k}\,.\,\mathbf{c}^{(D)}, \tag{5.31}$$

and this is all we require, because the phase function at points of vanishing structure factor is *defined* to be the linear extension of the diffraction pattern phase function to those points. Since (5.31) is explicitly linear in $\mathbf{k}$, it can be applied directly to $\mathbf{k}=\frac{1}{2}\mathbf{k}^{(D)}$ to give the required result.

Finally, we must establish that the phase function $\Phi_r(\mathbf{k})$ is linear, where r is a rotation through $2\pi/N$. For such a rotation (see Fig. 9)

$$n_j(r\mathbf{k})=n_{j-1}(\mathbf{k}) \tag{5.32}$$

and

$$r\mathbf{k}\,.\,\mathbf{c}^{(j)}=\mathbf{k}\,.\,\mathbf{c}^{(j-1)}, \tag{5.33}$$

again with the convention (5.25) for $\mathbf{c}^{(0)}$ and $n_0(\mathbf{k})$. This, however, immediately gives

$$S(r\mathbf{k})=\prod_{j=1}^{D}\,[1+(-1)^{n_{j-1}(\mathbf{k})}\exp(-i\mathbf{k}\,.\,\mathbf{c}^{(j-1)})]$$
$$=\prod_{j=0}^{D-1}\,[1+(-1)^{n_j(\mathbf{k})}\exp(-i\mathbf{k}\,.\,\mathbf{c}^{(j)})]. \tag{5.34}$$

Since this is the same* as the expression (5.27) for $S(m\mathbf{k})$, the same argument that established the linearity of $\Phi_m(\mathbf{k})$ establishes the linearity of $\Phi_r(\mathbf{k})$.

APPENDIX

Throughout this paper it is unnecessary to take the term 'space group' to mean anything more than an equivalence class of phase functions. The quasi-crystallographic space groups can, however, be given the algebraic structure of a group as follows:

(a) Take n vectors $\mathbf{v}^{(i)}$ that generate the lattice, in the sense that all lattice vectors $\mathbf{k}$ are integral linear combinations of the $\mathbf{v}^{(i)}$. Depending on circumstances,

* This simplification is a consequence of the particular mirror we chose to examine, but the conclusion, of course, does not depend on this choice.

one may take a generating set with the smallest possible value of n or prefer a set with larger n if it is more symmetric. Different choices of n will lead to different abstract groups.

(b) The n vectors $\mathbf{v}^{(i)}$ give a representation of the point group by n-dimensional matrices (of integers):

$$g\mathbf{v}^{(i)} = \sum \mathbf{v}^{(j)} D^{ji}(g). \qquad (A.1)$$

(c) Because the phase functions are linear to within additive integers, it is enough to specify their values at the n generating vectors. For each point-group operation g these values constitute an n-vector Φ_g with components

$$\Phi_g^{(i)} = \Phi_g(\mathbf{v}^{(i)}). \qquad (A.2)$$

(d) Because each component of a given phase-function vector Φ_g is determined only to within an additive integer, Φ_g can be represented by any member of the entire n-dimensional set S_g of vectors whose components differ from those of Φ_g by integers.

(e) Given any two representatives Φ_g and Φ_h from S_g and S_h, it follows from (3.6) that a vector from S_{gh} is given by

$$\Phi_{gh} = \Phi_g D(h) + \Phi_h. \qquad (A.3)$$

(f) Elements of the space group consist of ordered pairs (g, Φ_g), (g, Φ'_g), $(g, \Phi''_g), \ldots$ where g is any point-group element and $\Phi_g, \Phi'_g, \Phi''_g, \ldots$ are all the vectors in S_g. The combination law for two such pairs is the semidirect product

$$(g, \Phi_g)(h, \Phi_h) = (gh, \Phi_g D(h) + \Phi_h). \qquad (A.4)$$

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The Program *SAPI* and its Applications. I. Automatic Search of Pseudo-Systematic Extinction for Solving Superstructures

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Abstract

The name *SAPI* is an abbreviation of 'structure analysis programs with intelligent control'. It may also be read inversely as 'Institute of Physics, Academia Sinica'. *SAPI* is based on *MULTAN*80, but differs from it by a number of features. These will be described in a series of papers. The present paper describes an algorithm which can distinguish superstructures from ordinary structures by automatically discovering the pseudo-systematic extinction rule in reciprocal space. This algorithm enables *SAPI* to handle superstructures in a fully automatic way, leading to a complete solution in favourable cases.

Introduction

Superstructures are distinguished by their pseudo-translational symmetry, which leads to the effect of pseudo-systematic extinction, *i.e.* there exists two classes of reflections, one systematically strong, the

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