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Quasiperiodic tiling in two and three dimensions

J H Conway† and K M Knowles‡

† Department of Pure Mathematics and Mathematical Statistics, University of Cambridge, 16 Mill Lane, Cambridge CB2 1RX, UK

‡ Department of Metallurgy and Materials Science, University of Cambridge, Pembroke Street, Cambridge CB2 3QZ, UK

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Abstract. Algebraic criteria which allow the vertices of two- and three-dimensional Penrose tiling patterns to be specified are presented. The application of these criteria to the interpretation of electron microscope observations from quasicrystalline structures is discussed.

1. Introduction

Precipitates whose electron diffraction patterns exhibit icosahedral point symmetry have now been found in a variety of alloys, the most well known of which is the phase in Al-Mn originally discovered by Shechtman *et al* (1984). More recently, Bendersky (1985) has reported the existence of a further phase in the Al-Mn system whose electron diffraction patterns have a unique tenfold axis. Both these cases provide strong evidence for the existence of quasiperiodic structures in which there is long range order but no translational order. One possible interpretation of these structures is that they arise by a suitable atomic decoration of Penrose tiles in either two or three dimensions, as appropriate (see, for example, Mackay 1985, Henley 1985, Knowles *et al* 1985). However, in order to be able to compute electron diffraction patterns and high resolution electron micrographs for a given atomic decoration of the Penrose tiles, it is clearly necessary to have a method available for the generation of the vertices of a Penrose tiling pattern. Here, we derive suitable algebraic criteria for the generation of vertices in a three-dimensional Penrose tiling, where space is filled by two rhombohedra of equal sides but with angles of $\pm a\cos(1/\sqrt{5})$ i.e. 63.43° and 116.57° (Mackay 1982). We also provide algebraic criteria for generating vertices in a two-dimensional Penrose tiling in which space is filled with two rhombuses of equal sides but with angles of 72° and 144° (Gardner 1977). Finally, we comment on their application to electron microscope calculations of possible quasicrystalline structures.

2. Quasiperiodic tiling in three dimensions

We begin by defining six orthonormal vectors e_i, $i = 1$-6 spanning a six-dimensional space. These vectors can be identified as the rows of the unit 6×6 matrix

$$I=\begin{bmatrix}1&0&0&0&0&0\\0&1&0&0&0&0\\0&0&1&0&0&0\\0&0&0&1&0&0\\0&0&0&0&1&0\\0&0&0&0&0&1\end{bmatrix}=\begin{bmatrix}e_1\\e_2\\e_3\\e_4\\e_5\\e_6\end{bmatrix}.$$

Within this six-dimensional space, we further define two spaces V and W spanned by vectors which can be identified as the row vectors of the two matrices

$$V=\begin{bmatrix}\sqrt5&1&-1&-1&1&1\\1&\sqrt5&1&-1&-1&1\\-1&1&\sqrt5&1&-1&1\\-1&-1&1&\sqrt5&1&1\\1&-1&-1&1&\sqrt5&1\\1&1&1&1&1&\sqrt5\end{bmatrix}=\begin{bmatrix}V_1\\V_2\\V_3\\V_4\\V_5\\V_6\end{bmatrix}\tag{1}$$

and

$$W=\begin{bmatrix}-\sqrt5&1&-1&-1&1&1\\1&-\sqrt5&1&-1&-1&1\\-1&1&-\sqrt5&1&-1&1\\-1&-1&1&-\sqrt5&1&1\\1&-1&-1&1&-\sqrt5&1\\1&1&1&1&1&-\sqrt5\end{bmatrix}=\begin{bmatrix}W_1\\W_2\\W_3\\W_4\\W_5\\W_6\end{bmatrix}.\tag{2}$$

Each of these matrices is of rank three, i.e. only three of the six vectors defined in each space are required to span the space. Moreover, these two three-dimensional spaces within the six-dimensional space are orthogonal, since

$$VW=WV=0.$$

Within each space, the angle between the ith row vector and the kth row vector is $\pm a\cos(1/\sqrt5)$ (see also Elser 1985), so that the row vectors can be identified with vectors defining the vertices of icosahedra, as in figure 1. Each basis vector e_i in the six-dimensional space can now be written as

$$e_i=\frac{1}{2\sqrt5}(V_i-W_i)$$

and hence the e_i can be resolved into components in, or equivalently projections onto, the two spaces. We will call the projection onto W space of a vector e_i its elevation $E(e_i)$ and the projection onto V space its plan $P(e_i)$.

Consider now the projection onto W space of a six-dimensional cube centred at $[0,0,0,0,0,0]$ and with vertices at $[\pm\frac12, \pm\frac12, \pm\frac12, \pm\frac12, \pm\frac12, \pm\frac12]$. The projection of this cube is defined by the shape formed by the elevations of each of its 64 vertices. These elevations can be sorted into four distinct groups according to their size.

The twelve elevations with the largest moduli of $\tau/\sqrt2$ are defined by

$$\pm\frac{\tau}{2\sqrt5}W_i \qquad i=1\text{-}6 \tag{3a}$$

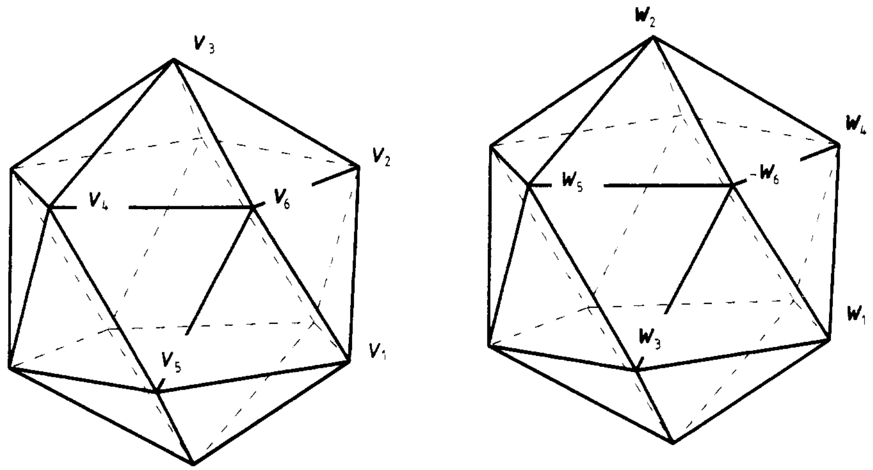


Figure 1. Icosahedra centred at the origin showing the relative orientation of the row vectors V_i and W_i, $i = 1$-6 spanning the two spaces V and W. The vectors are represented as vertices of these icosahedra.

where $\tau = (\sqrt{5}+1)/2$. One such elevation is

$$E(\tfrac{1}{2}, \tfrac{1}{2}, \tfrac{1}{2}, \tfrac{1}{2}, \tfrac{1}{2}, -\tfrac{1}{2}) = \frac{\tau}{2\sqrt{5}} W_6. \tag{3b}$$

The 20 next largest have moduli of $(0.3(\tau+2))^{1/2}$, such as

$$E(\tfrac{1}{2}, \tfrac{1}{2}, \tfrac{1}{2}, \tfrac{1}{2}, -\tfrac{1}{2}, -\tfrac{1}{2}) = \frac{\tau}{2\sqrt{5}}[\tau^2, \tau^{-1}, \tau^{-1}, \tau^2, -\tau^{-1}, -\tau]. \tag{4}$$

These two groups of elevations can be identified as defining the vertices at the fivefold and threefold axes respectively of a rhombic triacontahedron in W space centred at the origin. The remaining two groups of elevations divide into a group of 20 with moduli τ^{-1} $(0.3(\tau+2))^{1/2}$ and a group of 12 with moduli $\tau^{-1}/\sqrt{2}$. These two groups of elevations are vectors proportional to the threefold and fivefold axis vectors of the rhombic triacontahedron defined by the first groups of elevations, but lie within this rhombic triacontahedron.

We therefore have the result that the projection of a six-dimensional cube onto W, i.e. its elevation, is a rhombic triacontahedron. For the cube centred at [0, 0, 0, 0, 0, 0], the face centres of this rhombic triacontahedron are then expressible as the 15 vectors

$$\boldsymbol{h} = \pm\frac{1}{2}\frac{\tau}{2\sqrt{5}}(\boldsymbol{W}_i \pm \boldsymbol{W}_j) \qquad i \neq j \qquad i, j = 1\text{-}6 \tag{5}$$

and are vectors such as

$$\begin{aligned}
&\frac{\tau}{4\sqrt{5}}(\boldsymbol{W}_1 - \boldsymbol{W}_2) = \frac{\tau}{2\sqrt{5}}[-\tau, \tau, -1, 0, 1, 0] \\
&\frac{\tau}{4\sqrt{5}}(\boldsymbol{W}_1 + \boldsymbol{W}_3) = \frac{\tau}{2\sqrt{5}}[-\tau, 1, -\tau, 0, 0, 1] \\
&\frac{\tau}{4\sqrt{5}}(\boldsymbol{W}_1 - \boldsymbol{W}_6) = \frac{\tau}{2\sqrt{5}}[-\tau, 0, -1, -1, 0, \tau].
\end{aligned} \tag{6}$$

It follows that the condition that the elevation $\boldsymbol{Y}$ of a particular point $\boldsymbol{X}=[a, b, c, d, e, f]$ in the six-dimensional space lies within this rhombic triacontahedron is simply that

$$|\boldsymbol{X}\cdot\boldsymbol{h}|\leqslant\boldsymbol{h}\cdot\boldsymbol{h} \tag{7}$$

or equivalently that

$$|\boldsymbol{X}\cdot\boldsymbol{h}|<0.1(\tau+1)(\tau+2) \tag{8}$$

for each $\boldsymbol{h}$ defined by equation (5). The full set of 15 inequalities is obtained by cyclically rotating the first five coordinates of each of the three expressions on the right-hand side in equation (6).

These conditions on a given point $\boldsymbol{X}$ form the basis of the method we propose for generating sextuplets of integers which define vertices of a three-dimensional Penrose tiling.

Let L be the integer lattice in six-dimensional space shifted by an arbitrary vector $[a_0, b_0, c_0, d_0, e_0, f_0]$. A typical point on this integer lattice is then

$$\boldsymbol{X}=[a_0+u, b_0+v, c_0+w, d_0+x, e_0+y, f_0+z]$$

where u, v, w, x, y and z are integers. The vector $\boldsymbol{X}$ therefore defines the unit cube centred at $\boldsymbol{X}$. The elevation of this cube is then $\boldsymbol{Y}+R$. The origin is in this elevation if and only if $-\boldsymbol{Y}$ is within R, or equivalently if $\boldsymbol{Y}$ is within R, in which case equation (7) is satisfied for each $\boldsymbol{h}$ defined by equation (5).

The three-dimensional Penrose tiling may now be defined by stating that its vertices are the plans of the centres of those cubes whose elevations lie within R. The conditions for this to hold are that the inequalities in equation (8) be satisfied.

This has formed the basis of a computer program used to generate allowed sextuplets of integers by testing the vector $\boldsymbol{X}$ obtained by applying a fixed small shift $[a_0, b_0, c_0, d_0, e_0, f_0]$ with a_0, b_0, c_0, d_0, e_0 and $f_0 \ll 1$ to the integer lattice. These sextuplets define the vertices of acute and obtuse rhombohedra with angles of $\pm a\cos(1/\sqrt{5})$ which fill the three-dimensional Penrose tiling in a non-periodic manner. It is convenient to define these vertices in conventional three-dimensional coordinates by specifying step vectors $\boldsymbol{s}_i$, $i=1$–6, which are the projections of the $\boldsymbol{e}_i$ onto V. Suitable $\boldsymbol{s}_i$ are the rows of the matrix

$$\boldsymbol{S}=(2\tau+1)^{-1/2}\begin{bmatrix}1 & \tau & 0\\ 0 & 1 & \tau\\ 0 & -1 & \tau\\ 1 & -\tau & 0\\ \tau & 0 & -1\\ \tau & 0 & 1\end{bmatrix}=\begin{bmatrix}\boldsymbol{s}_1\\ \boldsymbol{s}_2\\ \boldsymbol{s}_3\\ \boldsymbol{s}_4\\ \boldsymbol{s}_5\\ \boldsymbol{s}_6\end{bmatrix}$$

and so a sextuplet of integers $[u, v, w, x, y, z]$ represents a vertex of the tiling at $u\boldsymbol{s}_1+v\boldsymbol{s}_2+w\boldsymbol{s}_3+x\boldsymbol{s}_4+y\boldsymbol{s}_5+z\boldsymbol{s}_6$. Since these $\boldsymbol{s}_i$ are also necessarily identifiable as being parallel to the fivefold axes of a suitable icosahedron, it is a simple matter to project the pattern down the fivefold axes, such as $\boldsymbol{s}_2$, threefold axes such as $\boldsymbol{s}_1+\boldsymbol{s}_2-\boldsymbol{s}_4$, twofold axes such as $\boldsymbol{s}_2+\boldsymbol{s}_3$ and mirror axes perpendicular to fivefold axes such as $\boldsymbol{s}_1+2\boldsymbol{s}_2-\boldsymbol{s}_4$. Formally, these axes in the tiling are not true symmetry axes, but since the power spectra FF^* from their Fourier transforms exhibit these symmetries (see also Duneau and Katz 1985, Elser 1986), it is convenient to refer to them as such. Figure 2 shows the projected positions of the vertices defining a three-dimensional Penrose tiling within a given 'box' for each of the axis types; in each case, the height of the 'box' along the

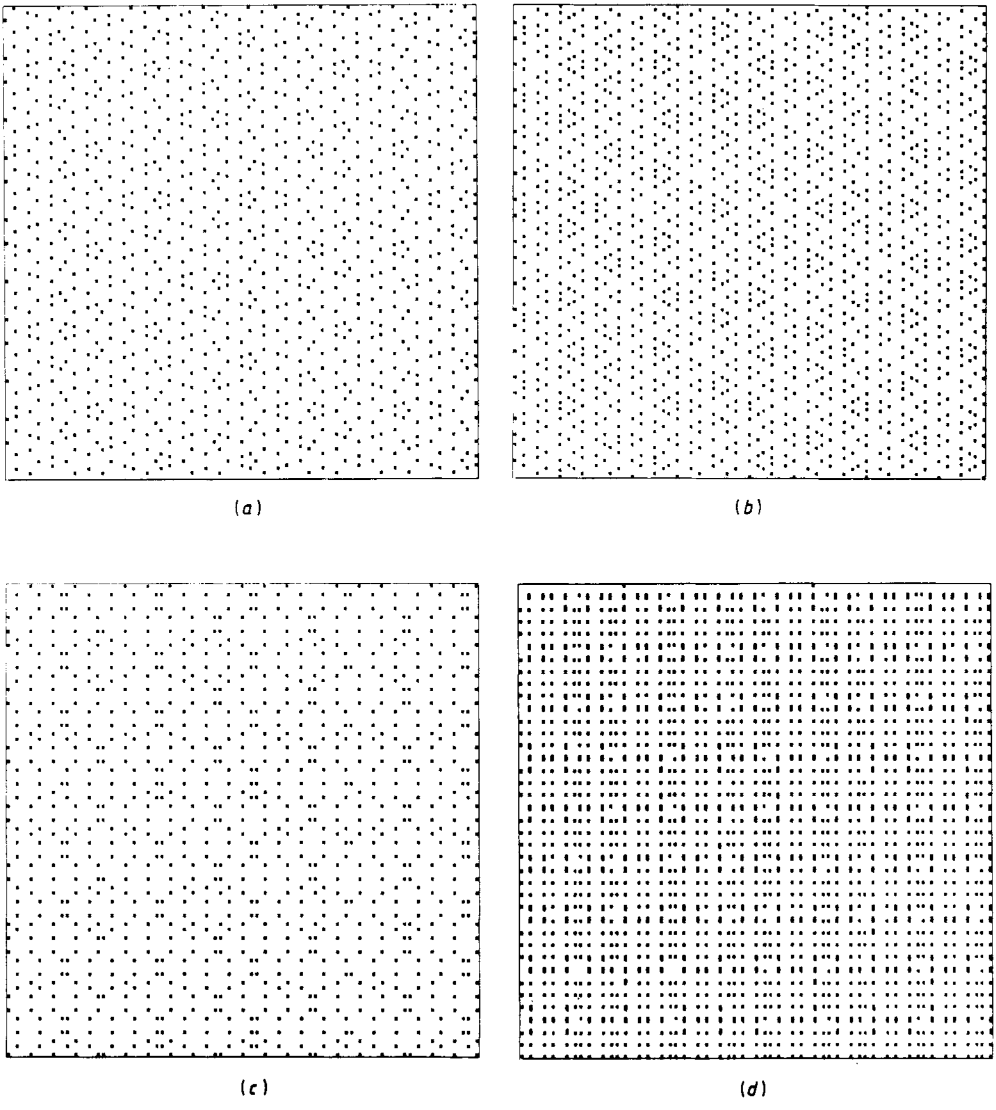


Figure 2. Projected positions of points defining the vertices of acute and obtuse rhombohedra in a 3D Penrose tiling down (a) a fivefold axis, (b) a threefold axis, (c) a twofold axis and (d) a mirror axis perpendicular to a fivefold axis. In each case, the vertices falling within a box of size $L \times L \times L/2$ are shown, where the square of side L is perpendicular to the axis of projection and the dimension of $L/2$ is along the axis of projection.

projection axis has been chosen to be half the width of the square dimension orthogonal to the projection axis.

3. Quasiperiodic tiling in two dimensions

For the two-dimensional Penrose tiling, in which space is filled aperiodically with two rhombuses with angles of 72° (thick rhombuses) and 144° (thin rhombuses), it is convenient to define five orthonormal vectors e_i, $i = 1$–5 spanning a five-dimensional space. These vectors can be identified as the rows of the unit 5×5 matrix.

Let L be the integer lattice in this space shifted by a vector $[a_0, b_0, c_0, d_0, e_0]$. A typical point on this integer lattice is then

$$X = [a, b, c, d, e] = [a_0 + u, b_0 + v, c_0 + w, d_0 + x, e_0 + y]$$

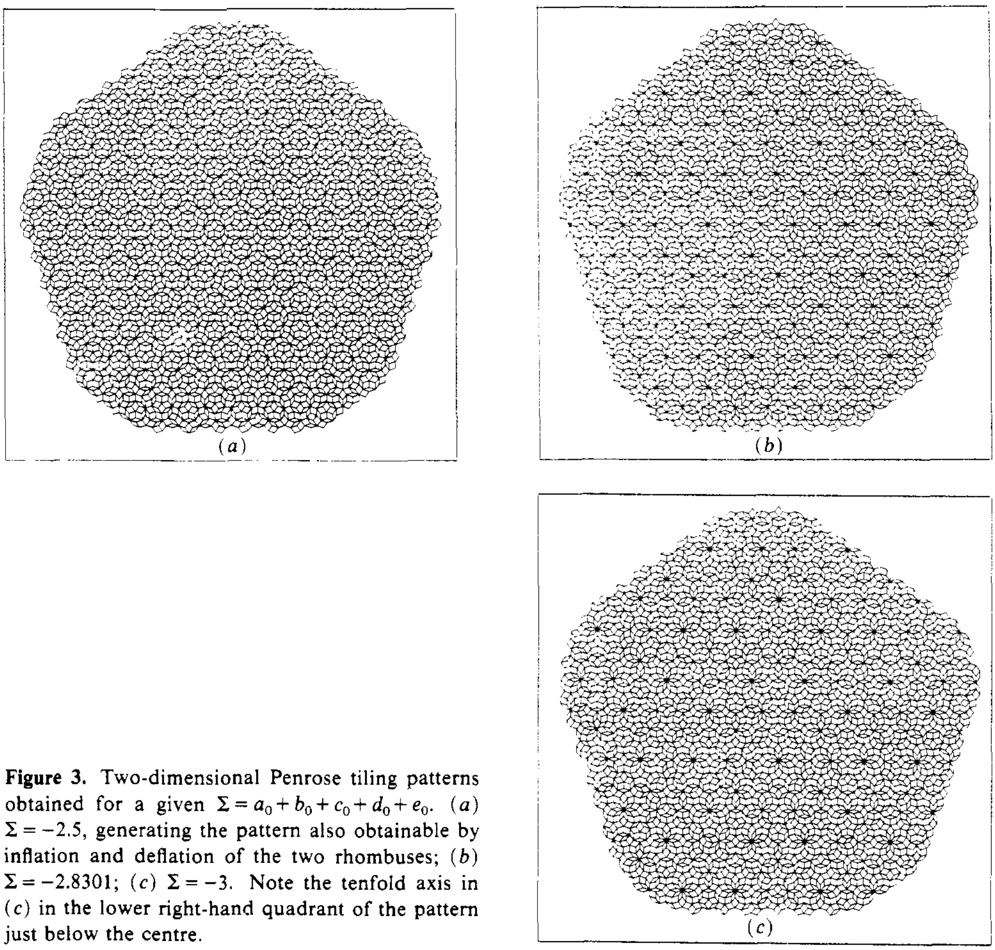
where u, v, w, x and y are integers. X then generates a vertex of the two-dimensional aperiodic tiling if and only if

(i) the modulus of its inner product with any cyclic permutation of $[\tau, 0, 1, 1, 0]$ is $\leqslant \tau\sqrt{5}/2$ and

(ii) the modulus of its inner product with any cyclic permutation of $[-\tau^{-1}, 1, 0, 0, 1]$ is $\leqslant \tau^2/2$.

Suitable step vectors are s_i, $i = 1$–5, cyclically defining the vertices of a regular pentagon from its centre.

In the two-dimensional case, it is also necessary to apply a sum condition that $a_0 + b_0 + c_0 + d_0 + e_0 = \frac{1}{2}(\mathrm{mod}\ 1)$ to create the non-periodic patterns discussed by de Bruijn (1981), which he terms AR (arrowed rhombus) patterns. In these patterns, de



(a) (b) (c)

Figure 3. Two-dimensional Penrose tiling patterns obtained for a given $\Sigma = a_0 + b_0 + c_0 + d_0 + e_0$. ($a$) $\Sigma = -2.5$, generating the pattern also obtainable by inflation and deflation of the two rhombuses; (b) $\Sigma = -2.8301$; (c) $\Sigma = -3$. Note the tenfold axis in (c) in the lower right-hand quadrant of the pattern just below the centre.

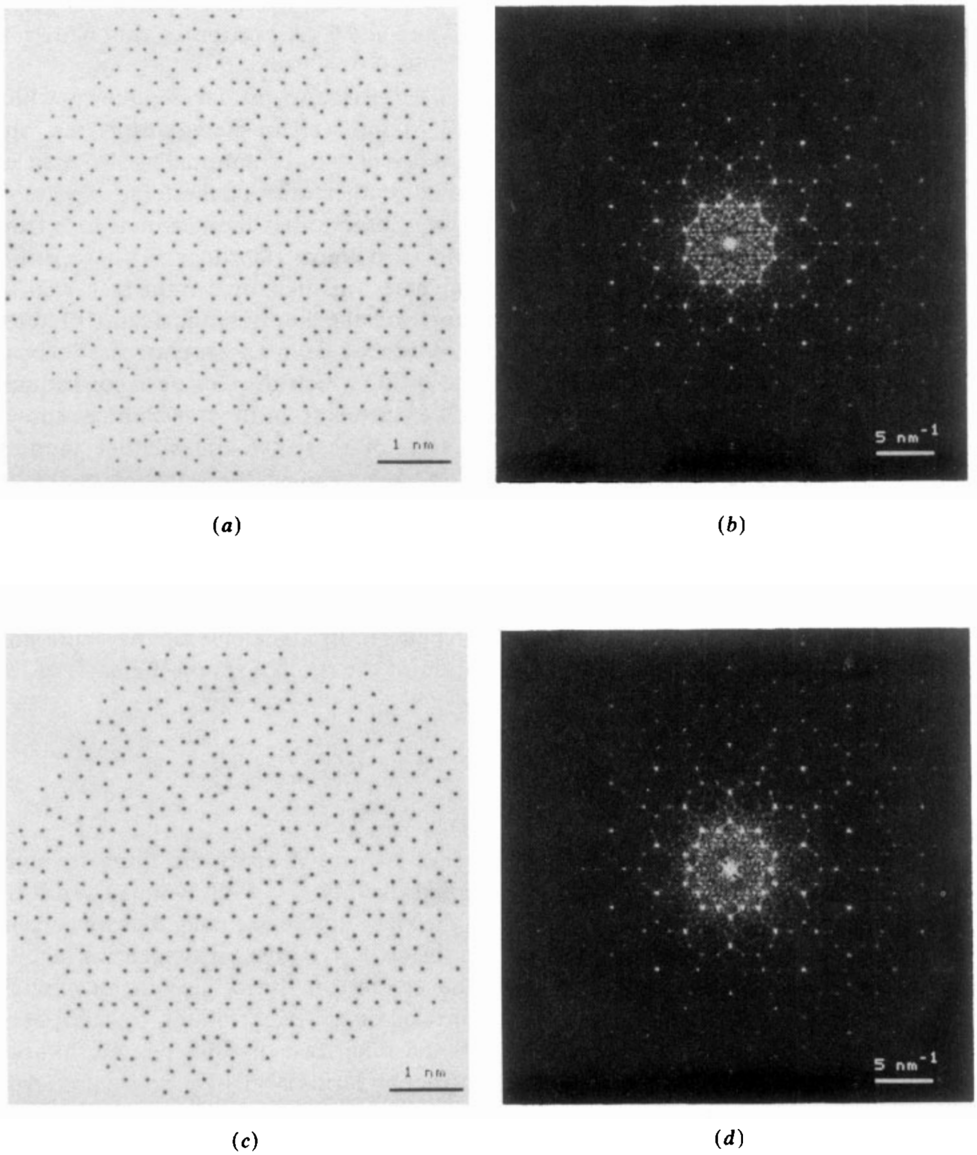


Figure 4. (a, c) 2D quasilattice models and (b, d) their associated power spectra for 500 kV electrons displayed on a logarithmic scale of intensity. In (a) and (c), aluminium atoms occupy the vertices of the patterns and the rhombus sides are the atom–atom distances in crystalline aluminium, 0.286 nm. For (a) and (c) $\Sigma = -2.5$ and for (b) and (d) $\Sigma = -3$.

Bruijn identified eight vertex types having coordination numbers between three and seven. Further features of this particular pattern are that the ratio of the number of thick rhombuses to the number of thin rhombuses in a portion of the pattern approaches τ as the area of the portion tends to infinity, and that for $a_0+b_0+c_0+e_0=-n-2.5$ for some integer n, the sum of the integers $u+v+w+x+y$ defining a particular vertex will be one of the integers $n+1$, $n+2$, $n+3$ and $n+4$. A portion of this pattern is shown in figure 3(a).

Relaxing the sum condition on $a_0+b_0+c_0+d_0+e_0$ also produces patterns which are aperiodic, such as those shown in figures 3(b) and 3(c). In such patterns, the ratio of the number of thick rhombuses to the number of thin rhombuses is also τ in an infinite portion of the tiling. While the detailed mathematics of these latter patterns will be discussed elsewhere (Conway 1986), we observe that they cannot arise from the inflation and deflation rules for producing AR patterns (Gardner 1977, de Bruijn 1981) and are instead distinct aperiodic 'universes' in their own right (see also de Bruijn 1981, Jaric 1986). The power spectra from the Fourier transforms of these patterns differ only on a fine scale from that produced from an AR pattern. This can be seen by a comparison of figures 4(b) and 4(d), which display on a logarithmic scale of intensity the power spectra for 500 kV electrons from the quasilattices shown in figures 4(a) and 4(c) respectively. For each of these two quasilattice models, aluminium atoms were placed at all the allowed vertices of the portions of the 2D patterns shown and the rhombus sides were taken to be equal to the atom-atom distance in crystalline aluminium, 0.286 nm. Although these models are physically unrealistic in that they permit aluminium-aluminium nearest-neighbour distances which are much too close, the similarity of figures 4(b) and 4(d) clearly demonstrates the potential difficulty of distinguishing between different pattern arrangements of the acute and obtuse rhombuses for a given atomic decoration of the rhombuses on the basis of the diffraction pattern intensities.

4. Discussion

The method we have proposed for the three-dimensional aperiodic tiling involves constructions similar to those proposed by Kramer and Neri (1984), Duneau and Katz (1985), Elser (1986) and Socolar *et al* (1985), the main difference being that we present our criteria for deciding whether a point lies inside a given region (which we take to be the elevation of the six-dimensional cube centred at the origin) in an explicit algebraic form suitable for generating portions of quasiperiodic tiling by computer. The criteria we have presented for the two-dimensional case are also related to those proposed by de Bruijn (1981) and discussed further by Jaric (1986). De Bruijn preferred to use the concept of pentagrids to define the tiling; however, the necessity of projecting from a five-dimensional space to a two-dimensional plane is a common feature.

Whichever method is used to produce the vertices defining the aperiodic tiling in either 2D or 3D, any material with a quasicrystalline structure must decorate the tiling with atoms in a suitable manner able to account for experimental observations. One approach to this has been to study the crystal structures of phases with similar compositions and, by appropriate atomic shuffles, decompose these structures into the two acute and obtuse rhombohedra from the 3D tiling (e.g. Mackay 1985, Henley 1985, Audier and Guyot 1986, Henley and Elser 1986). Alternatively, atomic decorations of the acute and obtuse rhombohedra have been suggested using density and packing considerations for hard spheres (Knowles *et al* 1985, Kimura *et al* 1986). In a companion paper (Knowles and Stobbs 1986), we show that by considering small volumes of quasicrystal with different atomic decorations, radically different x-ray and kinematical electron diffraction patterns can be obtained, just as in the atomic decoration of Bravais lattices in crystalline materials. This approach allows a way of eliminating models which would otherwise appear to be viable for a given alloy system, without recourse to lengthy image simulations of high resolution electron micrographs. However, such simulations are clearly necessary for atomic decorations which give reasonably good quantitative agreement with x-ray diffraction data where, in principle, the effects of double diffraction can be ignored, even for a quasicrystalline material. In these cases, the 3D quasicrystalline structure needs to be specified over appreciable areas, in order to minimise the edge effects in multislice calculations and to perform calculations for reasonable thicknesses of 10 nm or more.

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