

Statistical approach in cluster analysis of two-dimensional quasicrystals

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An analytical formula for the structure factor of Penrose tiling in the cluster approach was derived and tested. Probability distributions obtained for each Penrose position allow the number of different atoms that can decorate the cluster to be found. Calculations were performed in the average-unit-cell approach for Gummelt's cluster of 33 atoms, divided into three independent groups of atoms, and a kite cluster of 17 atoms, divided into seven independent groups.

1. Introduction

In quasicrystals, certain characteristic and frequently occurring groups of atoms called clusters can be found. A recent review of coverings of quasiperiodic sets was published by Kramer & Papadopolos (2003). The reader can find there references to many papers on this subject, among them also references to the most fundamental works of Steinhardt & Jeong (1996), Gummelt (1996) and Jeong & Steinhardt (1997), and many others: Baake *et al.* (1990), Duneau (1995), Janot (1997), Cotfas & Verger-Gaugry (1997), Urban (1998), Ben-Abraham & Gähler (1999), Kramer (1999), Gähler (2000), Gratias *et al.* (2000, 2001), Papadopolos & Kasner (2001), who have contributed enormously to the field of covering. It is possible to cover the entire quasicrystalline structure by some types of clusters. For instance, for Penrose rhombus tiling it is a set of atoms lying within a regular decagon called a cartwheel decagon which covers completely the whole structure. As some atoms belong to different neighbouring clusters, it is important to determine the ways clusters overlap. For the cartwheel decagons, matching rules were first introduced by Gummelt (1996). Gummelt's cluster consisting of 33 atoms is shown in Fig. 1. We also used a smaller cluster, called a 'kite cluster' with only 17 atoms, also marked in Fig. 1. Both clusters cover the rhombic Penrose tiling but with different degrees of covering (thickness of covering). Great overlap between the neighbouring clusters limits the possibility of decoration by different atoms. In that sense, Gummelt's cluster has much less freedom for decoration by different atoms than the kite cluster.

When calculating the diffraction pattern of quasicrystals, one should remember that 'the naive approach to Fourier theory of clusters fails: owing to overlap, the Fourier transform of a set of overlapping clusters cannot be expressed in terms of the Fourier transform of a single cluster together with the transformation of the quasiperiodic distribution of the centers of the clusters' (Kramer & Papadopolos, 2003, p. 18). In this paper, we calculate the probability distribution (over the

whole quasicrystalline structure) of individual atoms forming the cluster in an average-unit-cell approach (Wolny, 1998). These probabilities allow calculation of the structure factor and then the diffraction pattern for the studied quasicrystal. The analysis is conducted for some characteristic types of cluster decoration (for example, for non-decorated Penrose tiling). For these types, we calculate the formulas for structure factors. Finally, we discuss the applications of the obtained formulas in the determination of unknown quasicrystalline structure (with arbitrary decoration of the cluster) from a measured diffraction pattern.

In this paper, a statistical approach to the discussed structure is used. In the physical space it leads to the so-called average unit cell (Wolny, 1998; Wolny *et al.*, 2002; Kozakowski & Wolny, 2005). Such a cell represents the probability distribution of reduced atomic distances, *i.e.* the atomic distance with respect to the reference lattice. The reference lattice in two dimensions is a periodic set of parallel lines perpendicular to a chosen scattering vector \mathbf{k} , with a periodicity constant

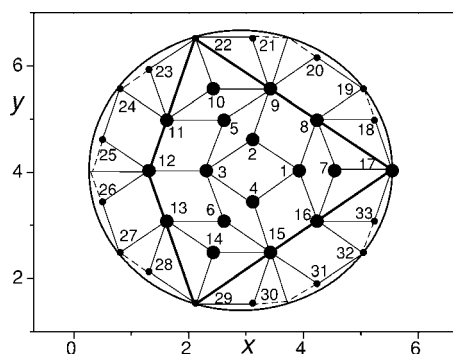


Figure 1
 Gummelt's cluster consisting of 33 atoms placed inside a regular decagon. The kite cluster consisting of 17 atoms (big filled circles) is also shown in the figure (thick lines). These clusters, in ten different orientations, cover the rhombic Penrose tiling (thin lines). The clusters presented in the figure are called [00001] clusters. The vector pointing from atom 1 to atom 17 is directed along the [00001] direction (the x direction in the figure).

equal to $\lambda = 2\pi/k$. The structure factor for the scattering vector \mathbf{k} and its higher harmonics are then given by the Fourier transform of the average unit cell. When raised up to higher dimensions, the average unit cell becomes an atomic surface (see also Fig. 2). Such interpretation of the atomic surface means that any point of this surface (in the perp-space) represents a particular combination of surrounding atoms in physical space. Similar interpretation of the atomic surface was also given by Gratias (2001). From this point of view, the two objects, the average unit cell in physical space and the atomic surface in perp-space, are fully equivalent. In the cut-and-project approach to quasicrystals, instead of the atomic surface one uses a window function equivalently. When covering the discrete point sets (vertex set of Penrose tiling), it is easier to perform any calculation of the structure factor in perp-space and that was done for 33/17 atom clusters. After the calculations in higher-dimensions, an oblique projection was used to write the final formula for the structure factor in physical space. This is because the physical space is more natural for the description of any decorations (Kozakowski & Wolny, 2005). Usually, the decorating atoms and their atomic surfaces look very complicated in perp-space and rather simple in physical space. The extension of the derived formula for the structure factor of the complete kite cluster (*i.e.* behind the 17-atom cluster) is straightforward in physical space only.

There is no mathematical proof for the covering of a vertex set of Penrose tiling by the 17-atom cluster used in this paper. However, such covering was checked numerically for several thousand atoms. Additionally, the obtained atomic surfaces for vertices fully cover the well known atomic surface for a vertex set of Penrose tiling. Finally, the derived formula for the diffraction peak intensities fully agrees with the calculated diffraction patterns for different subsets of atoms used for this checking.

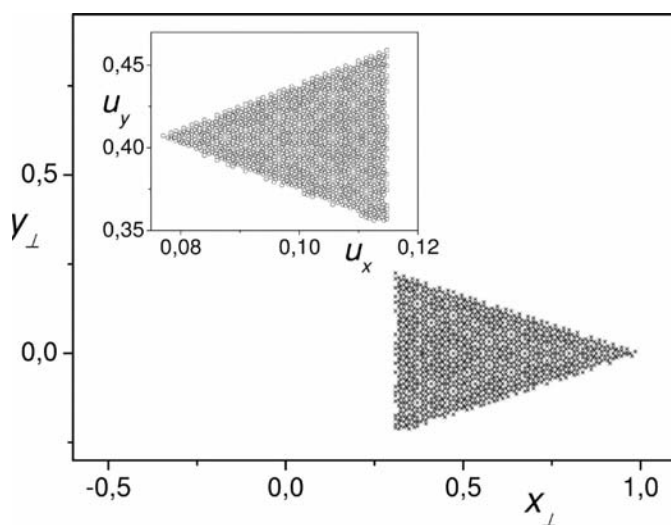


Figure 2
Average unit cell for atom 1 of the [00001] cluster shown in physical and perpendicular spaces. Open circles (physical space) and stars (perp-space) represent 1456 atoms used in the calculations. A uniform distribution of atomic positions is visible on both spaces.

2. Atoms in clusters – statistical approach

In this section, we assume that atoms are placed at the corners of rhombic Penrose tiling. For the discussed Gummelt and kite clusters, there are 33 and 17 atoms, respectively (Fig. 1). To calculate the structure factor, one needs to know the distribution of atomic positions for a particular cluster, either in physical space [average-unit-cell approach (Wolny, 1998)] or in perpendicular space on the atomic surface (higher-dimensional approach). As has already been shown (Wolny *et al.*, 2002; Kozakowski & Wolny, 2005), for perfect Penrose tiling these two approaches are completely equivalent. The average-unit-cell approach can be, however, easily extended to imperfect structures including phonons and phasons and some other defects. In this paper, we are dealing with perfect tilings only and the two approaches are used alternatively in an equivalent way. The calculated probability distributions in the inner (perp) and the physical spaces are shown in Fig. 2 for atom 1 of the kite cluster (Fig. 1). For these calculations, 1456 atomic clusters were used. The atomic positions in the average unit cell were plotted using open circles and using stars in the inner space. These two distributions have triangular shapes and correspond to one other. The average-unit-cell distribution can be obtained by oblique projection of the corresponding atomic surface (Steurer & Haibach, 1999; Cervellino & Steurer, 2002; Wolny *et al.*, 2002). Analytical calculations performed for atom 1 placed at the corner of the thick rhombus gives a triangular distribution as shown in Fig. 3. The area of the shadowed triangle (P_Δ , see also Appendix B) is τ^4 times smaller than the area of the triangle marked by 1 in Fig. 3 and it corresponds to the distribution of the vertex of the big rhombus in the rhombus Penrose tiling (Kozakowski & Wolny, 2005). This conclusion is not surprising as soon as one recognizes the similarity of the kite cluster to the τ^2 inflated Penrose tiling. The triangular distribution is obtained as a common part of a small pentagon (for atom 1 placed at $z = 1$) and all the other 16 atomic distributions appropriately shifted by $\Delta\mathbf{r}_\perp$ and Δz (Table 1). It can be shown that only four

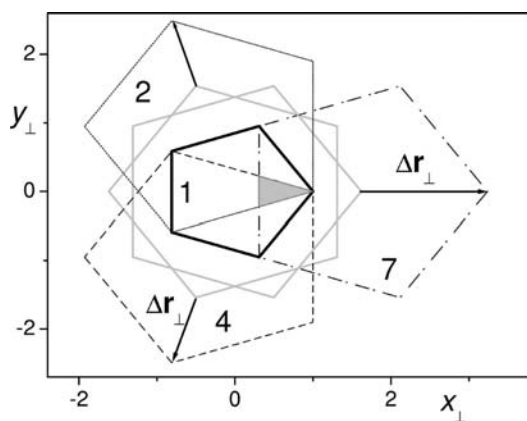


Figure 3
Distribution of atomic positions for atom 1 of the [00001] cluster. For rhombic tiling, the distribution is uniform in the triangle also marked by 1 (Kozakowski & Wolny, 2005). For the kite cluster, the distribution is described by the shaded triangle. The ratio of surfaces of those triangles equals τ^4 .

distributions (*i.e.* for four neighbouring atoms 1, 2, 4 and 7) fully determine the requested triangular area. The degree of covering (δ) is proportional to the ratio of ten differently oriented triangle areas, $10P_{\Delta}$, and the atomic surface area, P_{AS} , multiplied by the number of atoms in the cluster (N_C), which gives:

$$\delta = N_C \frac{10P_{\Delta}}{P_{AS}} = \frac{N_C}{\mu} \quad (1)$$

Symbol μ describes the effective number of atoms in the τ^2 inflated rhombic tiling and it is given by the equation $\mu = 5\tau + 3 \approx 11.09$ (this value is derived in the next section; see also Appendix B). For the kite cluster, this leads to $\delta_{17} \approx 1.53$. A similar approach to Gummelt's cluster, with 33 atoms, gives $\delta_{33} \approx 2.98$. It is obvious that the effective degree of covering is proportional to the number of atoms composing the cluster. For tiling by two rhombi, a thick one and a thin one, the effective thickness is equal to one. For covering by an infinitely big cluster, the degree of covering goes to infinity.

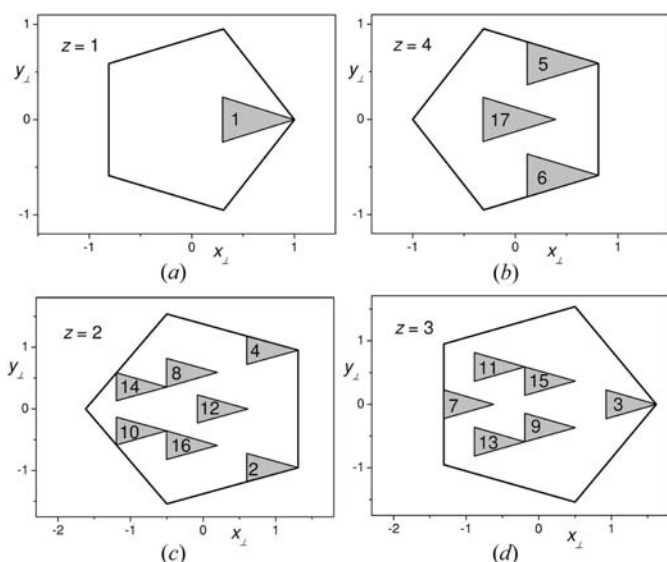


Figure 4 Probability distributions calculated in the perp-space (vertex atomic surfaces) for 17 atoms of the [00001] kite cluster. The shaded triangles represent the atomic surfaces of particular vertices of the cluster.

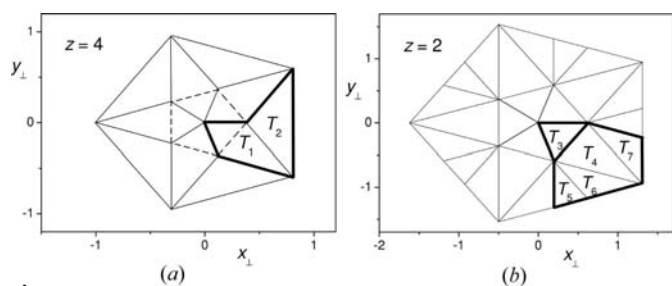


Figure 5 After averaging over ten equivalent directions, the obtained atomic surface splits into seven disjoint polygons T_i symmetrically arranged on the pentagons. Atoms belonging to different polygons never overlap for the whole Penrose tiling. For practical reasons, the tetragon T_1 has been divided into two triangles.

Knowing the probability distribution of individual atoms in physical space (average-unit-cell approach), one can extend this to higher dimensions (for more details, see Wolny *et al.*, 2002; Kozakowski & Wolny, 2005), getting the distribution on the atomic surface (Fig. 4). For all ten equivalent directions of the cluster and 17 different atoms, one covers the inner space with a thickness equal to δ_{17} . After tedious, but not very complicated, calculations, one obtains the following results. The atomic surface splits into seven polygons marked in Fig. 5 by T_i ($i = 1-7$). All of them, except for T_1 , are triangles. Fig. 5 shows two polygons, T_1 and T_2 , lying on the small pentagon ($z = 4$) of the atomic surface and five polygons, T_3-T_7 , lying on the big pentagon ($z = 2$). The T polygons consist of distributions of particular atoms, following the rules given in Table 3 in Appendix C. To describe the position in the perp-space, the notation in braces is used, which means that the coordinates are given in the units of $\mathbf{s} \equiv (s_x, s_y) = (\frac{1}{2}, \frac{1}{2}[\tau + 2]^{1/2})$. For any point written as $\{x_{\perp 1}, y_{\perp 1}\}$, the corresponding perp-space coordinates are equal to $x_{\perp} = x_{\perp 1}s_x$; $y_{\perp} = y_{\perp 1}s_y$.

The two chosen atoms belonging to different polygons T_i will never coincide in the Penrose tilings. This means that their positions can be occupied by different types of atoms. Even if T_6 and T_7 consist of atoms that do not overlap in the tiling, owing to symmetry reasons it can be supposed that the occupying atoms are of the same type. This means that the cluster can be decorated by seven (or six for symmetrical distributions) different atoms placed at Penrose positions.

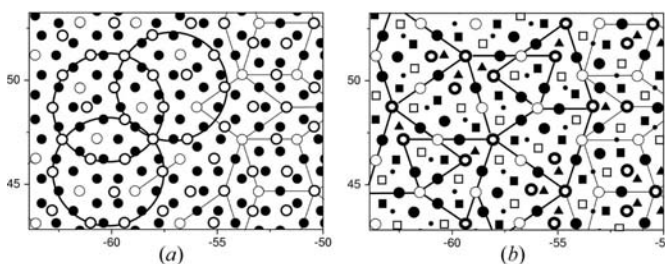


Figure 6 Decoration of Penrose tiling by different atoms. Only three different atoms can be used to cover the structure by Gummelt's clusters (a) and seven different atoms by kite clusters (b). The thin lines show the τ^2 inflated Penrose rhombic tiling, the thick lines covering by clusters.

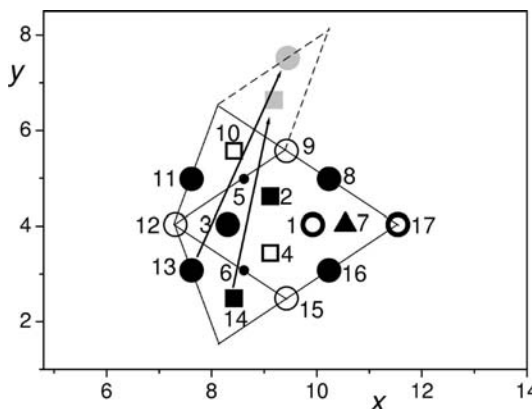


Figure 7 When shifting atoms 13 and 14 as is shown in the figure, one obtains two τ^2 inflated rhombi: thick and thin.

Similar calculations performed for Gummelt's cluster leads to only three different atoms as is shown in Fig. 6. In this case, the two polygons T_1 and T_2 (Fig. 5 for $z = 4$) combine into one polygon for a small pentagon. For a big pentagon, T_3 remains unchanged and the other four triangles, $T_4 - T_7$, are combined into a common polygon. One can easily see that as the cluster gets bigger the degree of covering increases but the number of different atoms that can be placed at the Penrose positions decreases. For an infinitely big cluster, there is only one type of atom that can be used for decoration of Penrose positions. Of course, there are infinitely many positions for different decorations of atoms behind the perfect Penrose positions. One gets more freedom for tiling the structure with two rhombi: a big and a small one, with edges τ^2 longer than the original tiling (Fig. 7). Such an artificial cluster consists of eight atoms decorating the thick rhombus and five atoms for the thin one. However, the number of thin rhombi is τ times smaller than the others, so the effective number of decorating atoms is equal to $\mu = 8 + 5/\tau \approx 11.09$, giving the thickness of covering equal to 1. There are common edges between the rhombi and from Fig. 7 it is evident that the number of different atoms is equal to nine. The inner atoms of thin rhombi (Nos. 10 and 14) can be completely different from the other seven decorating atoms of the thick rhombus. Finally, one can plot the dependence of the number of different decorating atoms *versus* the number of atoms forming the cluster (proportional to the degree of covering). For the three different clusters, an almost exponential dependence is observed (Fig. 8).

3. Diffraction patterns

To index the diffraction pattern of modulated structures, one has to choose some scattering vectors (we call them k vectors) for the main reflections and also some modulation vectors (called q vectors) for the satellite peaks. For Penrose tiling, one needs two k vectors, \mathbf{k}_1 and \mathbf{k}_2 , and also two q vectors, \mathbf{q}_1 and \mathbf{q}_2 (Wolny *et al.*, 2002; Kozakowski & Wolny, 2005). Vectors \mathbf{k}_1 and \mathbf{q}_1 are directed at an angle of 72° to the x axis, and vectors \mathbf{k}_2 and \mathbf{q}_2 are directed at an angle of -72° to the x axis. Equal lengths of q vectors are τ -times shorter than k vectors. For the rhombic Penrose tiling with edge lengths equal to 1:

$$|\mathbf{k}_1| = |\mathbf{k}_2| = \frac{4\pi}{5} \tau \equiv k_0 \approx 4.067; \tag{2}$$

$$|\mathbf{q}_1| = |\mathbf{q}_2| = \frac{4\pi}{5} = \frac{k_0}{\tau} \approx 2.513.$$

An arbitrary diffraction peak for scattering vector \mathbf{k} can then be expressed as a linear combination of \mathbf{k}_i and \mathbf{q}_i ($i = 1, 2$) with indices n_i and m_i appropriately and its components (k_x, k_y) are equal to:

$$k_x = k_0 c_1 \left(n_x + \frac{m_x}{\tau} \right) \tag{3}$$

$$k_y = k_0 s_1 \left(n_y + \frac{m_y}{\tau} \right), \tag{4}$$

where $c_1 = \cos(2\pi/5)$, $s_1 = \sin(2\pi/5)$,

$$\begin{aligned} n_x &\equiv n_1 + n_2, & m_x &\equiv m_1 + m_2, \\ n_y &\equiv n_1 - n_2, & m_y &\equiv m_1 - m_2. \end{aligned} \tag{5}$$

For the scattering vector given above, one can calculate the structure factor in an average unit-cell approach as follows (Wolny *et al.*, 2002; Kozakowski & Wolny, 2005):

$$F = \iiint P(u_1, u_2, v_1, v_2) \exp \left\{ ik_0 \left[n_1 u_1 + n_2 u_2 + \frac{1}{\tau} (m_1 v_1 + m_2 v_2) \right] \right\} du_1 du_2 dv_1 dv_2, \tag{6}$$

where $P(u_1, u_2, v_1, v_2)$ is a probability distribution that defines an average unit cell for the structure. For the Cartesian coordinates, one gets (u_x, u_y) and (v_x, v_y) , which leads to the following:

$$\begin{aligned} u_1 &= c_1 u_x + s_1 u_y; & v_1 &= c_1 v_x + s_1 v_y; \\ u_2 &= c_1 u_x - s_1 u_y; & v_2 &= c_1 v_x - s_1 v_y. \end{aligned} \tag{7}$$

Then one can write

$$F = \iiint P(u_x, u_y, v_x, v_y) \exp \left\{ ik_0 \left[c_1 \left(n_x u_x + m_x \frac{v_x}{\tau} \right) + s_1 \left(n_y u_y + m_y \frac{v_y}{\tau} \right) \right] \right\} du_x du_y dv_x dv_y. \tag{8}$$

Formula (8) is the same as (6) but written for Cartesian coordinates, which has a very practical meaning.

To calculate the structure factor, one has to know the probability distribution $P(u_x, u_y, v_x, v_y)$. For each atom of the 17-atom cluster, the distribution is non-zero inside the triangle Δ_{lj} , where $l = 1-17$ indicates the atom's number in the cluster and $j = 1-10$ describes the cluster orientation (see also Fig. 1). To get these triangular distributions, one has to project the distributions on the atomic surface onto physical space. As has already been shown (Kozakowski & Wolny, 2005), such an oblique projection for Penrose tiling is given by

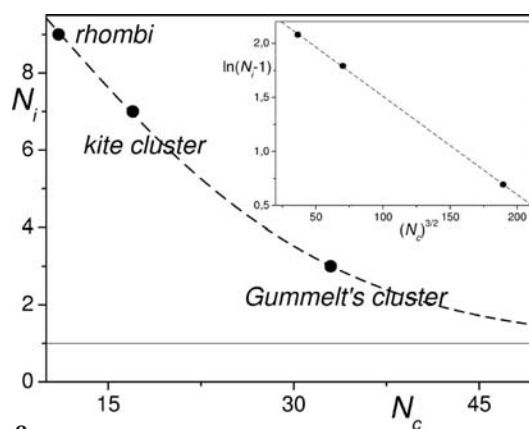


Figure 8 Number of different atoms *versus* number of atoms in the clusters. Three points corresponding to: Gummelt's cluster of 33 atoms (3 of them independent), kite cluster of 17 atoms (7 atoms independent) and two hypothetical rhombi (Fig. 7) with about 11 effective atoms (9 are independent) are shown in the figure. The dashed curve is only a guide to the eye, representing the exponential dependence. The inset is the same but shown on a different scale.

$$\mathbf{u} = \mathbf{A}\mathbf{r}_\perp,$$

where

$$\mathbf{u} \equiv \begin{pmatrix} u_x - 2z \\ u_y \end{pmatrix}; \quad \mathbf{r}_\perp \equiv \begin{pmatrix} x_\perp \\ y_\perp \end{pmatrix}; \quad \mathbf{A} = \begin{pmatrix} -1 & 0 \\ 0 & \tau^{-3} \end{pmatrix}. \quad (9)$$

The probability distribution is non-zero along the line

$$\mathbf{v} = -\tau^2 \mathbf{u}, \quad (10)$$

where

$$\mathbf{v} \equiv \begin{pmatrix} v_x + \tau z \\ v_y \end{pmatrix}.$$

Using the above, one can also write

$$F = \sum_{l=1}^{17} f_l \sum_{j=1}^{10} \exp(i\varphi_z) \iint_{\Delta_{lj}} \exp(i\mathbf{\kappa} \cdot \mathbf{u}) d^2u, \quad (11)$$

where

$$\varphi_z = z(\tau - 1)[k_x + m_x(3 - \tau)k_0] \quad (12)$$

$$\mathbf{\kappa} = \begin{pmatrix} k_x - m_x(2\tau - 1)c_1k_0 \\ k_y - m_y(2\tau - 1)s_1k_0 \end{pmatrix} \quad (13)$$

and f_l ($l = 1-17$) are the atomic form factors.

As all the distributions Δ_{lj} are organized in independent polygons T_s ($s = 1-7$) on the atomic surface, one can essentially reduce the formula for the structure factor:

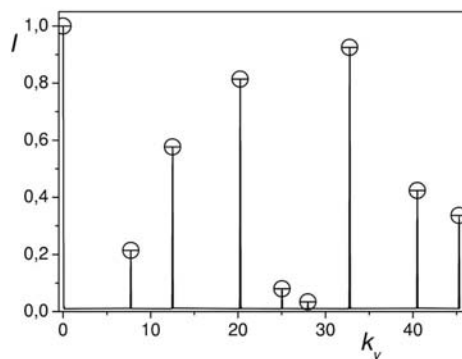
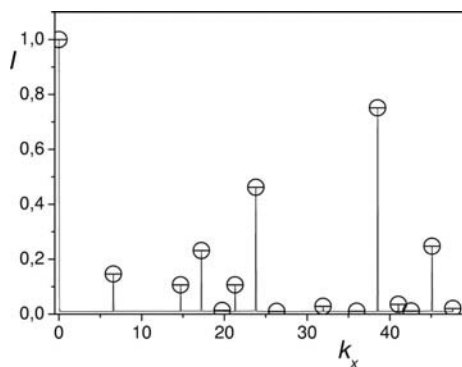


Figure 9

Diffraction patterns along the x (top) and y (bottom) directions calculated numerically for a set consisting of about 125 000 atoms (solid line) and from equation (14) (open circle with a bar) for the kite cluster decorated uniformly, $f_l = 1$ ($l = 1-17$), *i.e.* the first type of decoration. Full agreement between direct numerical calculations and analytical results obtained for the cluster's covering is observed.

$$F = \sum_{j=1}^5 B_j(\mathbf{k}), \quad (14)$$

where

$$B_j(\mathbf{k}) = \exp(i4\varphi_1) \sum_{l=1}^2 \Gamma_{lj}(\mathbf{\kappa}) + \exp(i2\varphi_1) \sum_{l=3}^7 \Gamma_{lj}(\mathbf{\kappa}) \quad (15)$$

$$\varphi_1 = \varphi_{z=1} = (\tau - 1)[k_x + m_x(3 - \tau)k_0] \quad (16)$$

$$\Gamma_{lj}(\mathbf{\kappa}) \equiv f_l \iint_{P_{lj}} \exp(i\mathbf{\kappa} \cdot \mathbf{u}) d^2u. \quad (17)$$

P_{lj} are the polygons T_l in j orientation ($j = 1-5$) when projected onto physical space.

The above formulas give the correct value of structure factor for any scattering vector given by (3) and (4). For a continuous variable of scattering vector, these formulas lead to the so-called envelope functions connecting diffraction peak intensities for a particular index of satellites (Wolny, 1998).

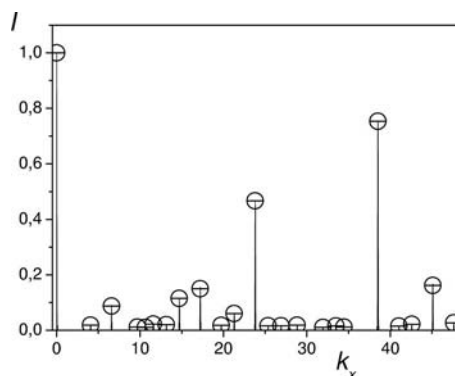


Figure 10

Diffraction pattern along the x direction for the second type of decoration, *i.e.* all the atoms belonging to the T_4 triangular distribution (numbered 3, 8, 11, 13 and 16) have zero amplitude of atomic scattering. The solid line is the diffraction pattern calculated for a big enough set of atoms, circles with bars represent results of the average-unit-cell calculations (14).

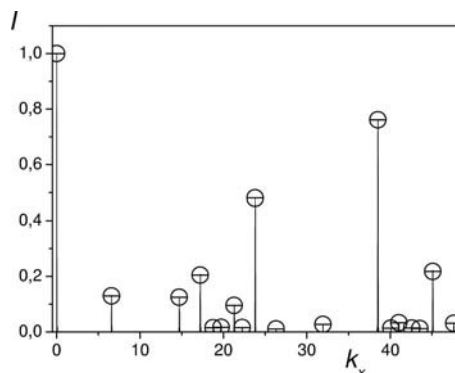


Figure 11

Diffraction pattern along the x direction for the third type of decoration, *i.e.* all the atoms belonging to the T_5 triangular distribution (numbered 7) have a zero amplitude of atomic scattering. The solid line is the diffraction pattern calculated for a big enough set of atoms, circles with bars represent results of the average-unit-cell calculations (14).

Several tests were performed to check the correctness of the derived formula for the structure factor (14). To do that, the diffraction patterns were calculated (from the proposed formula for the structure factor and also directly by Fourier transform using a big enough set of atoms) and compared for different decorations of Penrose tiling. Some of the results are shown in Figs. 9–11. To calculate the diffraction patterns, the following decorations of Penrose tiling were used:

(i) each vertex was decorated by a similar atom with the same atomic form factor, *i.e.* $f_l = 1$ ($l = 1$ –17);

(ii) five atoms numbered as 3, 8, 11, 13 and 16 belonging to the T_4 triangular distribution did not contribute to the diffraction pattern, *i.e.* $f_3 = f_8 = f_{11} = f_{13} = f_{16} = 0$, and for all the others the atomic form factors were equal to 1;

(iii) all the atomic form factors, except $f_7 = 0$, were equal to 1; atom 7 belonged to triangular distribution T_5 .

The diffraction pattern along the y direction is almost insensitive to the type of decoration used and it has been presented only once in Fig. 9. Observed agreement between peak intensities obtained in two different ways (direct Fourier transform and average unit-cell approach applied for clusters) fully supports the correctness of the presented idea.

4. Arbitrary decoration of cluster

Above, we have solved the problem of the allowed decoration of the corners of rhombi in the Penrose tiling. To reconstruct the rhombic Penrose tiling, it is sufficient to use a cluster of 17 atoms (kite cluster). To solve the problem of arbitrary decoration of the tiling, one needs to use the full kite cluster (Fig. 12), *i.e.* the cluster of 17 Penrose positions with four extra triangular regions on the two wings of the kite. In this figure, seven independent subregions are also shown. Decoration of individual subregions should be the same in the whole cluster. Any decorating atom can be included in the structure factor by an appropriate phase shift (given by the product $\mathbf{k} \cdot \mathbf{r}$) as

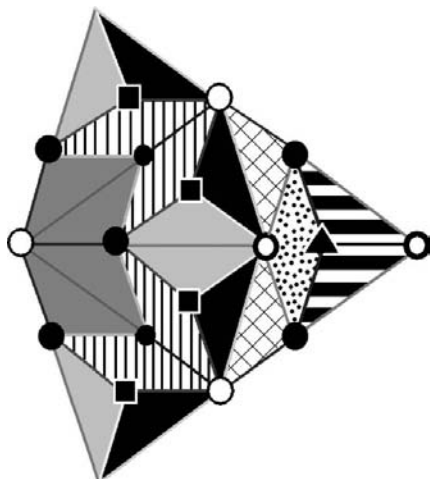


Figure 12

Kite cluster with seven regions marked that can be decorated independently by atoms.

was shown by Kozakowski & Wolny (2005) for decorated rhombi.

5. Conclusions

In this paper, for the first time, an analytical expression has been derived for the structure factor of Penrose tiling covered by atom clusters. Using a statistical approach (average unit-cell approach), it was possible to find the probability distributions of atoms decorating the cluster. Two clusters were thoroughly discussed: the Gummelt cluster, consisting of 33 atoms, and the kite cluster, of 17 atoms. Triangular probability distributions of positions of individual atoms have been found in the average unit cell and equivalently on the atomic surface. Those distributions calculated for all the decorating atoms and ten different orientations group into several disjoint regions (three for Gummelt's cluster and seven for the kite cluster). This allows us to find that for the smaller cluster there are seven independent atomic positions (reduced to six for a symmetrical cluster) that can be occupied by atoms independently. For Gummelt's cluster, the number of different decorating atoms is equal to three. Knowing the probability distributions of atomic positions, one can easily calculate the structure factor of the Penrose tiling in the cluster approach. Appropriate formulas were derived and compared with the direct numerical calculations for the complex of about 125000 atoms. Full agreement between the calculations (direct and the average-unit-cell approach) supports the correctness of the obtained formulas for the structure factor. For the kite cluster, seven types of regions can be found, which can be decorated independently. As the structure factor has been obtained in physical space, it is not very difficult to extend the derived formula to arbitrary decorated clusters. One has only to include the appropriate phase shifts for decorating atoms as was already shown by Kozakowski & Wolny (2005) for decorated rhombi.

Several tests have been performed for differently decorated Penrose tilings. The obtained diffraction patterns fully support the correctness of the ideas presented. One should notice that, even though the used decorations were completely different, the obtained diffraction patterns do not look much different (Figs 9–11). Only from the intensities of rather weak diffraction peaks along the x direction can one distinguish between different decorations. From the experimental data, it could be very difficult to solve the structure of quasicrystals without knowing the exact formula for the structure factor of arbitrary decorated clusters.

APPENDIX A

For any position given in a higher-dimensional space (five-dimensional) by $[a_1, a_2, a_3, a_4, a_5]$, one can calculate its perpendicular components using the following equations:

$$x_{\perp} = \frac{1}{2}[-\tau, \tau - 1, \tau - 1, -\tau, 2] \cdot [a_1, a_2, a_3, a_4, a_5] \quad (18)$$

$$y_{\perp} = \frac{(\tau+2)^{1/2}}{2}[\tau - 1, -1, 1, 1 - \tau, 0] \cdot [a_1, a_2, a_3, a_4, a_5]. \quad (19)$$

Table 1

Relative coordinates of 17 atoms placed at Penrose positions of the kite cluster [00001] shown in Fig. 1.

The origin coincides with the first atom. In square brackets, the higher-dimensional coordinates are indicated. In braces {}, the perp-space coordinates are given, $\Delta r_{\perp} \equiv \{x_{\perp}, y_{\perp}\}$ in the relative units of vector s .

Atom no.	D5 coordinates	Δz	Δr_{\perp}
1	[0,0,0,0,0]	0	{0, 0}
2	[0,1,0,0,0]	1	{ $\tau-1, -1$ }
3	[0,1,1,0,0]	2	{ $2\tau-2, 0$ }
4	[0,0,1,0,0]	1	{ $\tau-1, 1$ }
5	[1,1,1,0,0]	3	{ $\tau-2, \tau-1$ }
6	[0,1,1,1,0]	3	{ $\tau-2, 1-\tau$ }
7	[1,0,0,1,0]	2	{ $-2\tau, 0$ }
8	[1,0,0,0,0]	1	{ $-\tau, \tau-1$ }
9	[1,1,0,0,0]	2	{ $-1, \tau-2$ }
10	[1,1,0,0,-1]	1	{ $-3, \tau-2$ }
11	[1,1,1,0,-1]	2	{ $\tau-4, \tau-1$ }
12	[0,1,1,0,-1]	1	{ $2\tau-4, 0$ }
13	[0,1,1,1,-1]	2	{ $\tau-4, 1-\tau$ }
14	[0,0,1,1,-1]	1	{ $-3, 2-\tau$ }
15	[0,0,1,1,0]	2	{ $-1, 2-\tau$ }
16	[0,0,0,1,0]	1	{ $-\tau, 1-\tau$ }
17	[1,0,0,1,1]	3	{ $-2\tau+2, 0$ }

Table 2

Perp-space coordinates of vertices of triangular distributions for each of the 17 atoms of the kite cluster [00001].

Atom no.	Vertex 1	Vertex 2	Vertex 3
1	{2, 0}	{ $\tau-1, 2\tau-3$ }	{ $\tau-1, 3-2\tau$ }
2	{ $\tau+1, -1$ }	{ $2\tau-2, 2(1-\tau)$ }	{ $2\tau-2, 2(\tau-2)$ }
3	{ $2\tau, 0$ }	{ $\tau-3, 2\tau-3$ }	{ $3\tau-3, 3-2\tau$ }
4	{ $\tau+1, 1$ }	{ $2\tau-2, 2(\tau-1)$ }	{ $2\tau-2, 2(2-\tau)$ }
5	{ $\tau, \tau-1$ }	{ $2\tau-3, 3\tau-4$ }	{ $2\tau-3, 2-\tau$ }
6	{ $\tau, 1-\tau$ }	{ $2\tau-3, 4-3\tau$ }	{ $2\tau-3, \tau-2$ }
7	{ $2-2\tau, 0$ }	{ $-1-\tau, 2\tau-3$ }	{ $-1-\tau, 3-2\tau$ }
8	{ $2-\tau, \tau-1$ }	{ $-1, 3\tau-4$ }	{ $-1, 2-\tau$ }
9	{1, $\tau-2$ }	{ $\tau-2, 1-\tau$ }	{ $\tau-2, 3\tau-5$ }
10	{ $-1, \tau-2$ }	{ $\tau-4, 1-\tau$ }	{ $\tau-4, 3\tau-5$ }
11	{ $\tau-2, \tau-1$ }	{ $2\tau-5, 3\tau-4$ }	{ $2\tau-5, 2-\tau$ }
12	{ $2\tau-2, 0$ }	{ $3\tau-5, 2\tau-3$ }	{ $3\tau-5, 3-2\tau$ }
13	{ $\tau-2, 1-\tau$ }	{ $2\tau-5, 4-3\tau$ }	{ $2\tau-5, \tau-2$ }
14	{ $-1, 2-\tau$ }	{ $\tau-4, \tau-1$ }	{ $\tau-4, 5-3\tau$ }
15	{1, $2-\tau$ }	{ $\tau-2, \tau-1$ }	{ $\tau-2, 5-3\tau$ }
16	{ $2-\tau, 1-\tau$ }	{ $-1, 4-3\tau$ }	{ $-1, \tau-2$ }
17	{ $4-2\tau, 0$ }	{ $1-\tau, 2\tau-3$ }	{ $1-\tau, 3-2\tau$ }

If we assume that the first atom lies at the origin, the coordinates of all 17 atoms are given in Table 1.

APPENDIX B

Degree of covering

The probability distribution of atomic positions in the cluster [00001] has a triangular shape (Fig. 3) with vertices given in perp-space in Table 2 (in units of s).

The area of the triangles is then given by

$$P_{\Delta} = \frac{7\tau - 11}{4}(\tau + 2)^{1/2} \approx 0.15514. \quad (20)$$

The area of the big pentagon of the atomic surface is

Table 3

Perp-space positions of vertices of polygons T .

Distributions of 17 atoms of the kite cluster split into seven non-overlapping polygons that are triangles except for T_1 (a tetragon). For the simplicity of further calculations, the tetragon T_1 has also been split into two triangles T_{1A} and T_{1B} .

	Atomic numbers	Vertex 1	Vertex 2	Vertex 3
T_{1A}	1, 17	{0, 0}	{ $2(2-\tau), 0$ }	{ $2\tau-3, \tau-2$ }
T_{1B}		{ $\tau, 1-\tau$ }	{ $2(2-\tau), 0$ }	{ $2\tau-3, \tau-2$ }
T_2	5, 6	{ $2(2-\tau), 0$ }	{ $\tau, \tau-1$ }	{ $\tau, 1-\tau$ }
T_3	9, 12, 15	{0, 0}	{ $2(\tau-1), 0$ }	{ $2-\tau, 1-\tau$ }
T_4	3, 8, 11, 13, 16	{ $\tau+1, -1$ }	{ $2(\tau-1), 0$ }	{ $2-\tau, 1-\tau$ }
T_5	7	{ $2-\tau, 1-\tau$ }	{ $2-\tau, \tau-3$ }	{ $2(\tau-1), 2(1-\tau)$ }
T_6	2, 14	{ $2-\tau, 1-\tau$ }	{ $\tau+1, -1$ }	{ $2(\tau-1), 2(1-\tau)$ }
T_7	4, 10	{ $2(\tau-1), 0$ }	{ $\tau+1, 3-2\tau$ }	{ $\tau+1, -1$ }

$$P_B = \frac{(25 + 10 \times 5^{1/2})^{1/2}}{4}(\tau + 2) \approx 6.2247. \quad (21)$$

The area of the small pentagon $P_S = P_B/\tau^2$, so finally the area of the full atomic surface is

$$P_{AS} = 2(P_S + P_B) = 2\left(1 + \frac{1}{\tau^2}\right)P_B \approx 17.205. \quad (22)$$

The degree of covering is proportional to the number of different triangles [number of decorating atoms multiplied by the number of different orientations (10)] and is then given by

$$\delta_{17} = \frac{17 \times 10 \times P_{\Delta}}{P_{AS}} \approx 1.53; \quad \delta_{33} = \frac{33 \times 10 \times P_{\Delta}}{P_{AS}} \approx 2.98. \quad (23)$$

The values for the kite cluster δ_{17} and Gummelt's clusters δ_{33} are the same as obtained in the text.

APPENDIX C

For practical calculations, it is more convenient to split the tetragon T_1 into two triangles T_{1A} and T_{1B} . Then one obtains eight triangular distributions as given in Table 3. When projected onto physical space, there are eight triangles P_{ij} ($i = 1-8$) in five different orientations ($j = 1-5$). Fourier transform over a triangular area can be easily calculated using the following analytical formula:

$$\iint_P \exp(i\mathbf{\kappa} \cdot \mathbf{u}) d^2u = \frac{1}{\kappa_y} [D_{12}(E_2 - E_1) + D_{23}(E_3 - E_2) + D_{31}(E_1 - E_3)], \quad (24)$$

where P is a triangle with vertices at positions \mathbf{u}_p ($p = 1-3$);

$$D_{lm} = \frac{1}{\kappa_x + \kappa_y a_{lm}}, \quad E_p = \exp(i\mathbf{\kappa} \cdot \mathbf{u}_p) \quad (25)$$

and a_{lm} is a linear coefficient of the line going through vertices \mathbf{u}_l and \mathbf{u}_m .

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