

Structure factor for decorated Penrose tiling in physical space

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The structure factor for an arbitrarily decorated Penrose tiling has been calculated in the average unit cell description. The obtained formula uses only the physical coordinates of the atoms decorating a structure. The final equation can be easily extended so that it can describe the other physical properties of a structure. Its usefulness is demonstrated by its use in the Al–Ni–Co alloy structure-refinement process.

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1. Introduction

A stable decagonal Al–Co–Ni quasicrystal was identified by Tsai *et al.* (1989). Its phase diagram was thoroughly studied by Gödecke & Ellner (1996), and different phases (both decagonal and periodic approximants) were found by Zhang *et al.* (1997) and Ritsch *et al.* (1998). Penrose tiling is the best-known two-dimensional quasicrystals structure model which has proven to be an excellent starting point for the structure refinement of real decagonal quasicrystals (Steurer & Haibach, 1999; Steurer & Cervellino, 2001; Takakura *et al.*, 2001). This aperiodic tiling, discovered by Penrose (1974), was thoroughly studied by Grünbaum & Shephard (1987). There are many other types of aperiodic plane coverings which are also identified with the Penrose tiling (Baake *et al.*, 1991). The structural class of Penrose tilings used throughout this paper, for the purpose of the refinement process, is classified as the SMLD class (symmetry-conserving mutually derivable patterns). We have chosen rhombi as structural units. The fundamental properties of such rhomb coverings were derived by de Bruijn (1981).

In most cases the structure of a quasicrystal is analysed by means of the ‘cut and project’ method, which functions in high-dimensional space. The method has been widely discussed in many papers (de Bruijn, 1981; Kramer & Neri, 1984; Levine & Steinhardt, 1984; Duneau & Katz, 1985; Kalugin *et al.*, 1985; Elser, 1986; Janssen, 1988; Jagodzinski, 1991; Hof, 1995, 1997; Senechal, 1995). According to the ‘cut and project’ method, the analysis of the Penrose tiling involves the use of the five-dimensional space with the two-dimensional physical space and the three-dimensional inner space (perp-space). The structure is represented by its atomic surface which provides statistical information on high-dimensional atomic coordinates and which, in the case of the Penrose tiling, consists of two small and two large pentagons. The method provides a simple though abstract description of the quasicrystalline structure. It has some drawbacks, too. For instance, it is not easy to incorporate dynamic structural properties into

a structure model. Randomness or structural defects are other issues which are not easily accessible by this method (Elser, 1986; Baake *et al.*, 2003).

In this paper we outline calculations based on a statistical method called the average unit cell (AUC) approach (Wolny, 1998) which lead to the structure factor for two-dimensional Penrose tiling. The method described, after extension to the third physical (see §3.5) dimension, proves to be successful in a real quasicrystal structure refinement (Wolny *et al.*, 2008; Kuczera, Kozakowski *et al.*, 2010; Kuczera, Wolny & Steurer, 2010; Kuczera, Strzałka & Wolny, 2010). This paper is a general review of the theoretical work done on the development of the AUC approach for decagonal quasicrystals. The main concept of the paper is based on a theoretical work published in arxiv (Kozakowski & Wolny, 2005). Since then, the concept of the AUC has proven to be useful for various practical applications and, as the above was the only referral paper for a citation of the source of the AUC theory for the decagonal rhomb Penrose tiling, we have decided to modify it appropriately and publish it in print.

The multidimensional approach allows us to describe both modulated structures and quasicrystals by substituting atoms with their multidimensional equivalents, *i.e.* atomic surfaces. The paper shows that an AUC and an atomic surface are related by an oblique projection onto the physical space. Consequently, these two methods, in the case of perfect structures, can be considered as equivalents and they can be used interchangeably. The focal point, however, is the fact that a multidimensional approach assumes the structure to be periodic while the AUC approach does not require such an assumption.

There are examples of structures for which the multidimensional approach fails and the AUC does not. Such a structure is the Thue–Morse sequence (Wolny *et al.*, 2000; Wnęk *et al.*, 2001). The AUC approach makes it possible to conduct precise numerical calculations (with the use of integer numbers only) for an almost unlimited number of atoms. The resulting outcomes produce accurate values of fractal scale

factors of diffraction peaks, for both commensurate and incommensurate values of these factors.

Another example of a situation in which the multi-dimensional approach cannot be successfully applied is an analysis of a structure that produces a diffraction pattern containing not only an atomic component but also a continuous one. The paper by Orzechowski & Wolny (2007) shows how the AUC approach can deal with such a situation. The results give a new perspective on utilizing the entire diffraction pattern and not only Bragg peaks in a refinement process.

2. Average unit cell

An average unit cell is a concept which allows us to enforce periodicity on any structure, even on those which are not periodic or ordered. In order to define an AUC, a reference frame must be introduced. A reference frame is a set of parallel planes periodically arranged with the lattice constant λ . The position of any point placed along this lattice is measured with reference to the nearest leftward plane of the lattice. In other words, if the original atomic coordinates were denoted by r and their reference frame equivalents were denoted by u , then the following relationship would exist between these two sets of coordinates,

$$u_n \equiv r_n \bmod(\lambda). \quad (1)$$

In the case of periodic crystals, a reference frame simply defines a unit cell. When it comes to aperiodic structures such as quasicrystals, the coordinates of which are defined by a combination of an integer number and an irrational one, $\tau = (1 + 5^{1/2})/2$, the definition (1) is insufficient to give a meaningful description of the structure. In such cases it is preferable to describe a structure in probability terms, *i.e.* by stating the probability $P(u)$ of finding an atom within the interval stretched between coordinates ($u; u + du$). $P(u)$ defines an AUC, which is a probability distribution of atomic positions expressed with respect to a reference frame.

The AUC of a Fibonacci chain is a rectangular function (Senechal, 1995; Buczek *et al.*, 2005). In the case of Penrose tiling, the AUC consists of four pentagons (Wolny & Kozakowski, 2003). In Appendix A it is proven that there is a one-to-one relationship between the AUC and the atomic surface for a perfect Penrose tiling.

The crux of the method lies in the properties of the dot product $\mathbf{k} \cdot \mathbf{r}$, which is a part of the structure-factor phase. The dot product defines the projection of the entire structure in the direction of the wavevector. Consequently, the calculations are conducted for a one-dimensional structure stretched along this direction. Furthermore, a phase factor can be reduced by the multiplication of 2π . From the point of view of a diffraction analysis, this can be considered as a coordinate reduction to a single AUC. Such an approach allows us to determine the intensities of a periodic set of diffraction peaks positioned at multiples of \mathbf{k} . These peaks are often referred to as the main peaks. In order to calculate the intensities of peaks situated among the main ones, another wavevector must be introduced,

the modulated wavevector \mathbf{q} . The peaks associated with \mathbf{q} are often called the satellite peaks. Usually, for simplicity, we choose a parallel \mathbf{k} and \mathbf{q} . If, additionally, they are incommensurate, their linear combination can lead to almost any point (within experimental accuracy) situated along the chosen direction. The only problem underlying the analysis is the fact that two separate AUCs must be defined for both vectors \mathbf{k} and \mathbf{q} . In many cases, however, these two AUCs are related to each other and the relationship can be used in further calculations. The application of the AUC approach significantly simplifies numerical calculations.

For quasicrystals, such as the one-dimensional Fibonacci chain, two-dimensional SMLD Penrose tiling or decagonal and icosahedral structures, the relationship between AUCs for \mathbf{k} and \mathbf{q} vectors is linear (which is shown in the paper). As a result, the multidimensional integrals can be easily transformed into one-dimensional ones. The phase factors obtained from those integrals are constant for a particular structure; they do not change during the refinement process. All the calculations are conducted only within the physical space coordinates.

3. Derivation of the structure factor

3.1. Model assumptions

There are many structural approaches to the basic structure of decagonal quasicrystals. Even the most basic model, the Penrose SMLD class, can be described by clusters, rhombi, Robinson triangles or kites and darts (Baake *et al.*, 1991). We decided to base our calculations mainly on the rhombi model (and thus we use the term 'Penrose tiling' when referring to a SMLD class covered by rhombi) as this is the most commonly used one. However, in the further part of the paper, we introduce an AUC approach to the cluster model as well.

There are two types of rhombi: a thin and a thick one. Each of them can be found in ten variants rotated with respect to each other at an integer multiple of the angle $\pi/10$. If we assume the tenfold diffraction symmetry, we can focus our attention only on one pair of rhombi. The ones we selected as structural units are shown in Fig. 1. After choosing the framework, the structural units can be decorated. The position of an atom put into a rhombus is given in relation to the highlighted vertices. Additionally, we assumed that if an atom is put along a side of a rhombus, then there are only 0.5 atoms in the unit. If an atom is placed at a vertex, it is counted as a fraction proportional to the angle of the vertex given as a part of the full angle.

An AUC for any of these structural units turns out to be of a triangular shape (Fig. 2). The exact coordinates of these triangles' vertices are calculated in Appendix B.

During the derivation of the structure factor, to make the calculation simpler, we omit atomic factors as well as the Debye–Waller factors and the third periodic coordinate z of decorating atoms. All these factors will be taken into account in the final form of the structure factor.

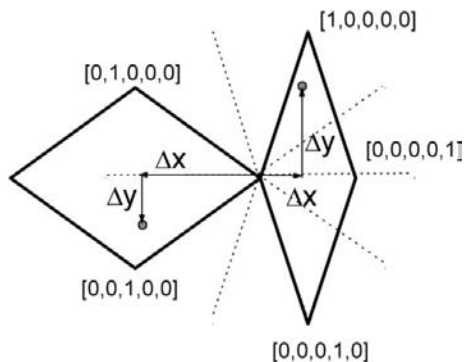


Figure 1
The rhombi selected as structural units. The coordinates of an atom decorating a rhombus are given in relation to the central point. Here they are denoted as $(\Delta x, \Delta y)$. In the background there are dotted lines which show the directions of the five-dimensional basis vectors projected onto the physical space. Their five-dimensional coordinates are given in square brackets.

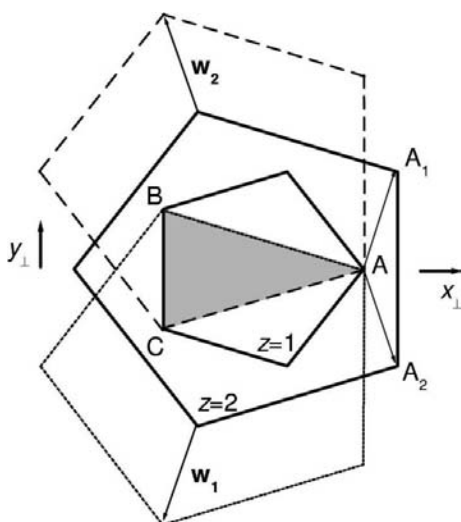


Figure 2
The procedure for obtaining the shape of the probability distribution for positions of thick rhombi. Details are provided in Appendix B. The shape found and subsequently projected onto the physical space becomes the AUC which is proven in Appendix A.

3.2. Reference frames

We use four different reference frames for positioning an atom of the Penrose tiling and three sets of reference scattering vectors for positioning diffraction peaks.

(i) *The natural, periodic frame.* According to the cut-and-project method (de Bruijn, 1981; Kramer & Neri, 1984; Levine & Steinhardt, 1984), a Penrose tiling can be represented by a set of regularly distributed points situated within the boundaries of a projection strip submerged in the five-dimensional space. The positions of a point can be expressed in such a situation as $\mathbf{R}_{[1]} = A[a_1, a_2, a_3, a_4, a_5]$ (rectangular parenthesis; $a_1 \dots a_5$, integer numbers). The definition of reciprocal space is straightforward: $\mathbf{K}_{[1]} = (2\pi/A)[h_1, h_2, h_3, h_4, h_5]$, where $h_1 \dots h_5$ are integer indexes. The symbol A represents the five-dimensional lattice constant. Although we have five dimen-

sions, only four main scattering vectors are needed to index the entire diffraction pattern. This assumption is proven in section (ii). The simplest choice for basis vectors would be $[1, 0, 0, 0, 0]$, $[0, 1, 0, 0, 0]$, $[0, 0, 1, 0, 0]$ and $[0, 0, 0, 1, 0]$. However, for the effective use of an AUC, we chose another basis vector: $\mathbf{K}_1 = (2\pi/A)[0, 0, -1, -1, 0]$; $\mathbf{K}_2 = (2\pi/A)[-1, -1, 0, 0, 0]$; $\mathbf{Q}_1 = (2\pi/A)[1, 0, 0, 0, 0]$ and $\mathbf{Q}_2 = (2\pi/A)[0, 0, 0, 1, 0]$. This choice will be explained in one of the subsequent sections.

(ii) *The frame stretching the external and internal spaces.* A periodic frame, defined above, can be rotated so that two of its axes encompass the physical (external) space, and the remaining three the perpendicular (internal) space. In such a case the position vector $\mathbf{R}_{[1]}$ is defined as $\mathbf{R}_{[1]} = \{\mathbf{r}_{||}, \mathbf{r}_{\perp}\} = \{x, y, x_{\perp}, y_{\perp}, z_{\perp}\}$ and the scattering vector is defined as $\mathbf{K}_{[1]} = \{\mathbf{k}_{||}, \mathbf{k}_{\perp}\} = \{k_x, k_y, k_{x_{\perp}}, k_{y_{\perp}}, k_{z_{\perp}}\}$. The symbol ‘||’ or lack of a subscript indicates the physical coordinates and the symbol ‘ \perp ’ indicates the perpendicular ones.

The transition matrix \mathbf{T} for both direct and reciprocal spaces is

$$\mathbf{T} = \left(\frac{2}{5}\right)^{1/2} \begin{bmatrix} c_1 & c_2 & c_3 & c_4 & c_5 \\ s_1 & s_2 & s_3 & s_4 & s_5 \\ c_2 & c_4 & c_6 & c_8 & c_{10} \\ s_2 & s_4 & s_6 & s_8 & s_{10} \\ 1/(2^{1/2}) & 1/(2^{1/2}) & 1/(2^{1/2}) & 1/(2^{1/2}) & 1/(2^{1/2}) \end{bmatrix} \quad (2)$$

where $c_j = \cos(2\pi j/5)$, $s_j = \sin(2\pi j/5)$. We obtain new coordinates by calculating them as $\mathbf{R}_{[1]} = \mathbf{TR}_{[1]}$ and $\mathbf{K}_{[1]} = \mathbf{TK}_{[1]}$.

It can be easily noticed that every multiple of a vector $(2\pi/A)[1, 1, 1, 1, 1]$ always leads to the same point $\mathbf{k} = (0, 0)$. One of the coordinates of the periodic frame is then redundant. We chose to eliminate the fifth one, *i.e.* $h_5 = 0$, and therefore we only use four of them to index the entire set of diffraction peaks.

By means of the introduced transition matrix, we can establish a relationship between the five-dimensional lattice constant A and the length of a rhombus side a . It is well known that the Penrose tiling is built of thick and thin rhombi. The positions of their vertices are the result of a projection of five-dimensional points, lying within a projection strip, on the physical space. After a projection, every two neighbouring points, *i.e.* the ones which are separated by the distance A , become vertices of a rhombus. This leads to the relationship $A = a(5/2)^{1/2}$. In every further equation, A will be substituted by this outcome.

The transition matrix can also be used to calculate the physical and perpendicular coordinates of vectors $\mathbf{K}_1, \mathbf{K}_2, \mathbf{Q}_1, \mathbf{Q}_2$ introduced in the previous section. The outcome reads

$$\begin{aligned} \mathbf{K}_1 &= (4\pi/5a)\{c_1\tau, s_1\tau, c_2(\tau-1), s_2(\tau-1), -1\}, \\ \mathbf{K}_2 &= (4\pi/5a)\{c_1\tau, -s_1\tau, c_2(\tau-1), -s_2(\tau-1), -1\}, \\ \mathbf{Q}_1 &= (4\pi/5a)\{c_1, s_1, c_2, s_2, 1/2\}, \\ \mathbf{Q}_2 &= (4\pi/5a)\{c_1, -s_1, c_2, -s_2, 1/2\}. \end{aligned} \quad (3)$$

The ‘{ }’ subscript indexes are skipped.

The physical coordinates of these vectors are the basis vectors we use to index a diffraction pattern. They are

$$\begin{aligned} \mathbf{k}_1 &= (4\pi\tau/5a)(c_1, s_1), & \mathbf{k}_2 &= (4\pi\tau/5a)(c_1, -s_1), \\ \mathbf{q}_1 &= (4\pi/5a)(c_1, s_1), & \mathbf{q}_2 &= (4\pi/5a)(c_1, -s_1). \end{aligned} \quad (4)$$

The lengths of \mathbf{k}_1 and \mathbf{k}_2 are of equal value. We denote it as k_0 ,

$$k_0 \equiv |\mathbf{k}_1| = |\mathbf{k}_2| = (4\pi\tau/5a) \simeq 4.067/a. \quad (5)$$

The same holds true for \mathbf{q}_1 and \mathbf{q}_2 , although their length is τ times shorter than k_0 ,

$$q_0 \cong |\mathbf{q}_1| = |\mathbf{q}_2| = k_0/\tau. \quad (6)$$

Other properties of these vectors are:

- (a) \mathbf{k}_1 and \mathbf{q}_1 are parallel and the same holds for \mathbf{k}_2 and \mathbf{q}_2 ;
- (b) the angle between \mathbf{k}_1 and \mathbf{k}_2 is $4\pi/5$.

(iii) *Average unit cell frame.* The reciprocal vector basis consists of vectors defined in the previous section, *i.e.* $\mathbf{k}_1, \mathbf{k}_2, \mathbf{q}_1, \mathbf{q}_2$. Vectors \mathbf{k}_1 and \mathbf{k}_2 are called the main vectors and \mathbf{q}_1 and \mathbf{q}_2 are vectors of modulation.

According to the theory on modulated structures, the length of the vector of modulation \mathbf{q} must be related to the structure modulation. It is also practical to choose such a \mathbf{q} so that it is parallel to the \mathbf{k} vector. The basis chosen meets these conditions. The position of any diffraction peak is the linear combination of these vectors,

$$\mathbf{k} = n_1\mathbf{k}_1 + m_1\mathbf{q}_1 + n_2\mathbf{k}_2 + m_2\mathbf{q}_2.$$

Symbols n_1, n_2, m_1 and m_2 are diffraction indexes which are used in the AUC approach.

An average unit cell based on these vectors would be highly impractical to manage. It would be unintuitive to give atoms' coordinates in an oblique reference frame. Therefore, for the purpose of the construction of an AUC, we converted the reciprocal vector basis into the Cartesian reference frame, in which the coordinates k_x and k_y of the \mathbf{k} vector are equal to

$$\begin{aligned} k_x &= k_0c_1(n_1 + n_2) + q_0c_1(m_1 + m_2), \\ k_y &= k_0s_1(n_1 - n_2) + q_0s_1(m_1 - m_2). \end{aligned} \quad (7)$$

In such a situation the average unit cell frame is defined by four lattice constants,

$$\begin{aligned} \lambda_{ux} &= 2\pi/(k_0c_1), & \lambda_{vx} &= 2\pi/(q_0c_1), \\ \lambda_{uy} &= 2\pi/(k_0s_1), & \lambda_{vy} &= 2\pi/(q_0s_1). \end{aligned}$$

The position of an atom can be expressed either by (u_x, u_y) coordinates ($0 \leq u_x < \lambda_{ux}$ and $0 \leq u_y < \lambda_{uy}$) or by (v_x, v_y) coordinates ($0 \leq v_x < \lambda_{vx}$ and $0 \leq v_y < \lambda_{vy}$). Furthermore, these two pairs of coordinates are not independent of each other. As proven in Appendix A, when an atom assumes the position (u_x, u_y) then its (v_x, v_y) coordinates are equal to

$$v_x = -\tau^2 u_x + c_x \quad \text{and} \quad v_y = -\tau^2 u_y + c_y.$$

The constants c_x and c_y depend on the position of the origin of the reference frame. The density function stretched over these coordinates is the AUC of an examined quasicrystal: $P(u_x, u_y)$.

(iv) *Rhombi frame.* The main purpose of the structure analysis is to find the positions of atoms decorating the

structural units. In our case they are a thick and a thin rhombus. Fig. 1 shows the rhombi we have assumed as unit structures. The coordinates $(\Delta x, \Delta y)$ of any decorating atom are given with reference to the highlighted points. There is an obvious relationship between the coordinates of an atom decorating a rhombus and the corresponding coordinates of the probability distribution associated with this atom. If we move an atom from the origin and the displacement is equal to $(\Delta x, \Delta y)$, then the probability function will move within the boundaries of an AUC along the vector $(\Delta u_x, \Delta u_y) = (\Delta x, \Delta y)$ unless $\Delta x > \lambda_{ux}$ or $\Delta y > \lambda_{uy}$. In such a situation

$$(\Delta u_x, \Delta u_y) = (\Delta x - \alpha\lambda_{ux}, \Delta y - \alpha\lambda_{uy}), \quad (8)$$

where α is an integer satisfying the condition $0 \leq u_x < \lambda_{ux}$ and $0 \leq u_y < \lambda_{uy}$.

3.3. Structure factor for perfect decagonal quasicrystals: a general case, the AUC approach

The structure factor for any set of points reads

$$F(\mathbf{k}) = \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{j=1}^N \exp(i\mathbf{r}_j \cdot \mathbf{k}), \quad (9)$$

where \mathbf{r}_j is the position vector of the j th atom and N is the total number of atoms.

As already pointed out, in the case of decagonal quasicrystals, the scattering vector \mathbf{k} reads: $\mathbf{k} = n_1\mathbf{k}_1 + m_1\mathbf{q}_1 + n_2\mathbf{k}_2 + m_2\mathbf{q}_2$. The exponent of (9) is then equal to

$$\mathbf{r}_j \cdot \mathbf{k} = \mathbf{r}_j \cdot (n_1\mathbf{k}_1 + n_2\mathbf{k}_2 + m_1\mathbf{q}_1 + m_2\mathbf{q}_2). \quad (10)$$

After a projection of the scattering vectors on the Cartesian frame the dot product reads

$$\begin{aligned} \mathbf{r}_j \cdot \mathbf{k} &= (n_1 + n_2)x_j k_0 c_1 + (n_1 - n_2)y_j k_0 s_1 \\ &+ (m_1 + m_2)x_j q_0 c_1 + (m_1 - m_2)y_j q_0 s_1, \end{aligned} \quad (11)$$

where $\mathbf{r}_j = (x_j, y_j)$.

It is worth noticing that the calculation of the dot product $\mathbf{r} \cdot \mathbf{k}$ leads to the projection of a position vector on the directions of the basis scattering vectors. Thus, for every scattering vector we can conduct separate one-dimensional calculations, *i.e.* use a one-dimensional reference frame.

To make use of the AUC approach, we express y_j and x_j by four new coordinates,

$$\begin{aligned} x_j &= u_{xj} + \alpha_{ux}\lambda_{ux}, & \lambda_{ux} &= 2\pi/(k_0c_1), \\ x_j &= v_{xj} + \alpha_{vx}\lambda_{vx}, & \lambda_{vx} &= 2\pi/(q_0c_1), \\ y_j &= u_{yj} + \alpha_{uy}\lambda_{uy}, & \lambda_{uy} &= 2\pi/(k_0s_1), \\ y_j &= v_{yj} + \alpha_{vy}\lambda_{vy}, & \lambda_{vy} &= 2\pi/(q_0s_1). \end{aligned} \quad (12)$$

where $\alpha_{ux}, \alpha_{uy}, \alpha_{vx}, \alpha_{vy}$ are integer numbers.

The dot product then reads

$$\begin{aligned} \mathbf{r}_j \cdot \mathbf{k} &= n_x(u_{xj} + \alpha_{ux}\lambda_{ux})k_0c_1 + n_y(u_{yj} + \alpha_{uy}\lambda_{uy})k_0s_1 \\ &+ m_x(v_{xj} + \alpha_{vx}\lambda_{vx})q_0c_1 + m_y(v_{yj} + \alpha_{vy}\lambda_{vy})q_0s_1, \end{aligned}$$

which is equal to

$$\mathbf{r}_j \cdot \mathbf{k} = n_x u_{xj} k_0 c_1 + n_y u_{yj} k_0 s_1 + m_x v_j q_0 c_1 + m_y v_j q_0 s_1 + 2\pi(\alpha_{ux} + \alpha_{uy} + \alpha_{vx} + \alpha_{vy}). \quad (13)$$

The obtained result is then inserted into (9). Additionally, the relationship $q_0 = k_0/\tau$ is used and the integer multiple of 2π is neglected. The resulting formula is

$$F(\mathbf{k}) = \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{j=1}^N \exp \left\{ ik_0 \left[n_x c_1 u_{xj} + n_y s_1 u_{yj} + \frac{1}{\tau} (m_x c_1 v_{xj} + m_y s_1 v_{yj}) \right] \right\}. \quad (14)$$

Since the coordinates are limited by the size of the AUC, the summation can be replaced by an appropriate integration over the AUC [a strict mathematical justification of this step can be found in Cervellino *et al.* (2002)],

$$F(\mathbf{k}) = \int_0^{\lambda_{ux}} \int_0^{\lambda_{vx}} \int_0^{\lambda_{uy}} \int_0^{\lambda_{vy}} P(u_x, u_y, v_x, v_y) \times \exp \left\{ ik_0 \left[n_x c_1 u_x + n_y s_1 u_y + \frac{1}{\tau} (m_x c_1 v_x + m_y s_1 v_y) \right] \right\} \times du_x du_y dv_x dv_y. \quad (15)$$

As has already been mentioned, a relationship exists between coordinates $v_x(u_x)$ and $v_y(u_y)$. A strict derivation of these formulas can be found in Appendix A. The results are

$$v_x = -\tau^2 u_x + a_x \quad \text{and} \quad v_y = -\tau^2 u_y. \quad (16)$$

The constant coefficient a_x could be omitted if the origin of the reference frame ($V_x U_x$) was appropriately positioned. Let us introduce u_{x0} and v_{x0} shift parameters which move the origin in such a way that the relationship $v_x(u_x)$ can be written as $v_x = -\tau^2 u_x$. Making use of these two equations and the shift parameters along with the integration

$$\int_0^{\lambda_{vx}} \int_0^{\lambda_{vy}} P(u_x, u_y, v_x, v_y) dv_x dv_y = P(u_x, u_y),$$

we obtain

$$F(\mathbf{k}) = \int_0^{\lambda_{ux}} \int_0^{\lambda_{uy}} P(u_x, u_y) \times \exp \left\{ ik_0 \left[(n_x - \tau m_x) c_1 u_x + (n_y - \tau m_y) s_1 u_y - c_1 \left(n_x u_{x0} + \frac{1}{\tau} m_x v_{x0} \right) \right] \right\} du_x du_y. \quad (17)$$

After introducing new variables

$$\begin{aligned} \chi_x &= (n_x - m_x \tau) \cdot k_0 c_1 \\ \chi_y &= (n_y - m_y \tau) \cdot k_0 s_1 \\ \varphi_0 &= c_1 \left(n_x u_{x0} + \frac{1}{\tau} m_x v_{x0} \right), \end{aligned} \quad (18)$$

the formula reads

$$F(\chi_x, \chi_y) = \int_0^{\lambda_{ux}} \int_0^{\lambda_{uy}} P(u_x, u_y) \exp[i(\chi_x u_x + \chi_y u_y - \varphi_0)] du_x du_y. \quad (19)$$

For Penrose tiling, $P(u_x, u_y)$ is represented by a probability distribution consisting of four pentagonal areas for which the function P assumes a constant value. There is a strict relationship between these pentagons and the atomic surface. One can be converted into the other by an oblique projection. The calculations leading to this relationship are provided in Appendix A. The resulting AUC, unlike the atomic surface, is asymmetric. In order to perform any symmetrical operation, regularity must be given back to the distribution. This is achieved by introducing new re-scaled coordinates. The final results must, however, be scaled back to their original proportion.

Appendix A also gives the exact formula for φ_0 . Its value depends on the relative distance between four pentagons. If we numbered the pentagons according to their z_{\perp} coordinate (*i.e.* $j = 1$ and 4 for the thin ones and $j = 2$ and 3 for the thick ones) then we could rewrite (19) as

$$F(\chi_x, \chi_y) = \sum_{j=1}^4 \int_0^{\lambda_{ux}} \int_0^{\lambda_{uy}} P_j(u_x, u_y) \exp[i(\chi_x u_x + \chi_y u_y - \varphi_{j0})] du_x du_y, \quad (20)$$

with $\varphi_{j0} = j(2\pi/5a)(-2n_x + m_x)$. Equation (20) provides the structure factor for the perfect Penrose tiling.

3.4. Structure factor for freely decorated Penrose tiling

Equation (20) needs only slight modification to allow it to describe freely decorated Penrose tilings. The procedure is as follows.

(a) Two elementary units: one thick and one thin rhombus are selected from the perfect Penrose tiling. They are shown in Fig. 1.

(b) An AUC is calculated for each of these units. Their shape is triangular. The coordinates of these distributions' vertices and the method for extracting them is presented in Appendix B. The probability distribution for thick rhombi is denoted by Δ_L and by Δ_S for thin ones.

(c) There are ten variants of each unit structure. We obtain their probability distributions by rotating the one found for the unit structures. As in the case of the perfect Penrose tiling, the AUC is not symmetrical. Therefore, to make the rotation significant, the distribution is stretched so it becomes regular; it is then rotated and finally the original proportions are given back to the first one by the inverse operation. To show that a distribution is dependent on the rotation, symbols assigned to the distribution probability are extended to $\Delta_L(\alpha)$ and $\Delta_S(\alpha)$, where α is an integer multiple of $2\pi/5$.

(d) A shift of an atom from the frame's origin [the frame is introduced in §3.2(iv)] is taken into consideration by multiplying the structure factor by the phase factor $\exp(i\mathbf{k}\Delta\mathbf{r})$. The shift vector is denoted by $\Delta\mathbf{r}_{L_n}(\alpha)$ for an n th atom decorating a thick rhombus; it is $\Delta\mathbf{r}_{S_n}(\alpha)$ for an equivalent of a thin rhombus. α indicates that, along with distributions, the positions of decorating atoms must be rotated as well.

(e) If an atom is placed along a rhombus's side or in its vertex, only a fraction p of this atom is included (see §3.1) in

the structure-factor calculations. The notation for the n th atom is p_{L_n} (for a thick rhombus) and p_{S_n} (for a thin one).

(f) Finally, the overall structure factor is the sum of structure factors given for each atom decorating the structure units.

(g) To simplify the calculation, only the real part of the structure factor is taken into account. This is possible as an AUC for a Penrose tiling is an even function (*i.e.* inversion is a pseudo-symmetric element of the tiling). The final form of the structure factor is

$$F(\mathbf{k}) = \text{re} \left[\sum_{n=1}^{n_L} F_{L_n}(\mathbf{k}) + \sum_{n=1}^{n_S} F_{S_n}(\mathbf{k}) \right], \quad (21)$$

where n_L and n_S are the numbers of atoms decorating the thick and thin rhombus and F_{L_n} and F_{S_n} are structure factors for the n th atom associated with these structural units. They are equal to

$$F_{L_n}(\mathbf{k}) = p_{L_n} \sum_{\alpha=0}^4 T_L(\mathbf{k}, \alpha) \exp[i\Delta\mathbf{r}_{L_n}(\alpha) \cdot \mathbf{k}], \quad (22)$$

$$F_{S_n}(\mathbf{k}) = p_{S_n} \sum_{\alpha=0}^4 T_S(\mathbf{k}, \alpha) \exp[i\Delta\mathbf{r}_{S_n}(\alpha) \cdot \mathbf{k}], \quad (23)$$

where

$$T_{L,S}(\mathbf{k}, \alpha) = \int \int_{\Delta_{L,S}(\alpha)} \exp[i(\chi_x u_x + \chi_y u_y - \varphi_0)] du_x du_y, \quad (24)$$

$$\varphi_0 = (2\pi/5a)(-2n_x + m_x).$$

Values of the Fourier transformations of triangular distributions are discussed in Appendix C.

3.5. Structure factor for the refinement process

The structure factor as given above is appropriate only for model numerical structures. It needs to be extended in order for it to be used in a refinement process. The following discussion applies to the n th atom of any structure unit. Factors which must be included in the Al–Ni–Co quasicrystals structure-factor equation are as follows.

(a) The occupation probability, p_{sof}^n .

(b) If the quasicrystalline sample is a mixture of transition metals TM and a light metal (such as Al), then the concentration coefficients used are p_{TM} for the transition metal and $p_{\text{Al}} = 1 - p_{\text{TM}}$ for Al.

(c) The atomic form factors for TM and Al, f_{TM}^n and f_{Al}^n .

(d) The average atomic form factor is a combination of all the above listed factors,

$$f_n = p_{\text{sof}}^n [p_{\text{TM}}^n f_{\text{TM}}^n + (1 - p_{\text{TM}}^n) f_{\text{Al}}^n]. \quad (25)$$

(e) The Debye–Waller factor D_L ,

$$D_n = \exp[-(1/16\pi^2)(k_x^2 + k_y^2)b_{xy}^n - (1/16\pi^2)k_z^2 b_z^n], \quad (26)$$

where b_{xy} is the average displacement parameter in the quasiperiodic plane and b_z is the displacement parameter in the c direction.

(f) The z coordinate. Decagonal quasicrystals are periodic along the third physical dimension ‘ z ’. There are two or four layers (Steurer & Cervellino, 2001; Takakura *et al.*, 2001)

which when projected onto the XY plane form the Penrose tiling. If we denote the period as c , then this additional dimension can be inserted into the structure factor by multiplying it by $\exp(il\xi)$, where l is a diffraction index and ξ is a fraction of c .

(g) The phason Debye–Waller factor D_{Ph} ,

$$D_{\text{Ph}} = \exp[-(1/16\pi^2)(k_{\perp x}^2 + k_{\perp y}^2)b_{\text{Ph}}], \quad (27)$$

where b_{Ph} is the phason displacement parameter.

After the application of all these factors, the final form of the structure factor for a thick rhombus reads

$$F_{L_n}(\mathbf{k}) = D_{\text{ph}} p_{L_n} f_n D_n \sum_{\alpha=0}^4 T_L(\mathbf{k}, \alpha) \exp[i\Delta\mathbf{r}_{L_n}(\alpha) \cdot \mathbf{k} + l\xi]. \quad (28)$$

For a thin rhombus the final outcome is similar.

3.6. Structure refinement of $\text{Al}_{72}\text{Ni}_{20}\text{Co}_8$

The theory presented has been used to refine the well known (Takakura *et al.*, 2001; Cervellino *et al.*, 2002) Al–Ni–Co structure model. The results are discussed by Wolny *et al.* (2008) in detail. Here we present only the final outcome.

The unit structures of the Penrose tiling were divided three times with obedience to the inflation rules. An atom is put at every position from the zeroth, first, second and third division. To fulfill the density restriction, additional atoms were put at several positions of the fourth division. In total, we used 65 decorating atoms.

The optimization was performed on a set of 449 distinct reflections (Takakura *et al.*, 2001). Atoms decorating the structure units were divided into 19 groups. This division is shown in Fig. 3. For each group we optimized a shift from Penrose tiling positions in the quasiperiodic plane (D_x, D_y), the occupation probability for vertices, the concentration of TM atoms and two components of the Debye–Waller factor. We obtained an R factor of 8.0% and an R_w factor of 6.1%. The resulting $F_{\text{obs}}/F_{\text{calc}}$ graph is shown in Fig. 4. In total, 92 parameters were refined. The refined shift parameters are very small (of the order of 1% of the lattice constant) which stems from the fact that atomic positions are very close to the initial coordinates of the Penrose tiling. The resulting structure has

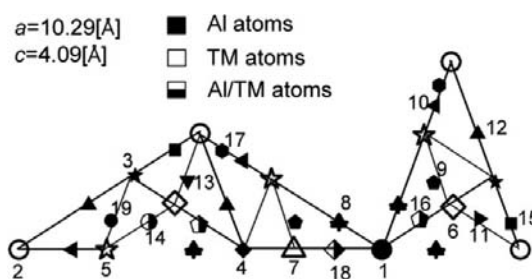


Figure 3 The initial decoration for the refinement procedure for the $\text{Al}_{72}\text{Ni}_{20}\text{Co}_8$ structure. Atoms were divided into 19 groups. Each group is represented by a different symbol. TM is either Ni or Co. The figure presents results more thoroughly discussed by Wolny *et al.* (2008).

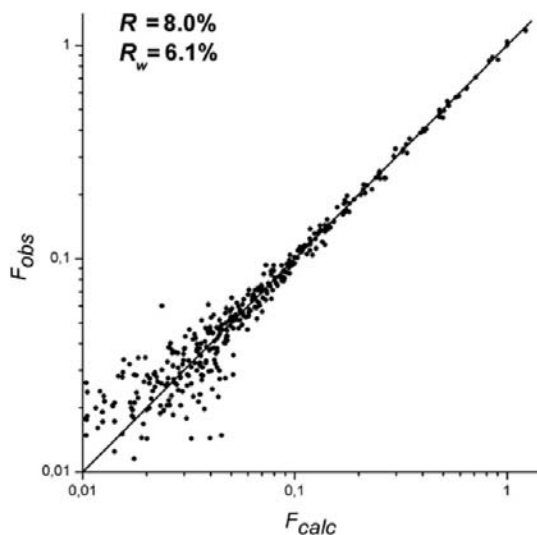


Figure 4

The amplitude of the structure factor observed in the experiment (F_{obs}) versus the calculated one (F_{calc}) for the $\text{Al}_{72}\text{Ni}_{20}\text{Co}_8$ model based on the AUC approach. The figure presents results more thoroughly discussed by Wolny *et al.* (2008).

the exact chemical composition of $\text{Al}_{72}\text{TM}_{28}$. Our model also gives good density values. The refined structure has a point density of 0.0663 \AA^{-3} and an overall density of 3.89 g cm^{-3} .

Recently, the AUC approach was successfully used to refine the structures of other decagonal phases reported in the Al–Ni–Co system, including the so-called superstructure type I phase, also known as the Edagawa phase (Kuczera, Kozakowski *et al.*, 2010; Kuczera, Wolny & Steurer, 2010). No other qualitative structure analysis of the Edagawa phase has been performed yet. The first attempt at the application of this method to Amman tiling, *i.e.* the three-dimensional generalization of the Penrose tiling, also looks very promising (Kuczera, Strzałka & Wolny, 2010).

4. Penrose tiling cluster model

The method for deriving a structure factor based on the AUC approach, as described in the previous sections, is a universal one. It can be applied to any type of structure (periodic, aperiodic, random) and to any model of the Penrose tiling. Having a few different models of the same structure gives us a chance to compare their results, study the differences or incorporate the most significant conclusions stemming from them in the final model of the examined structure. In this section the main points leading to the derivation of the structure factor for the Penrose tiling will be repeated for a cluster model of this quasicrystalline structure.

A cluster that is mostly associated with the Penrose tiling is Petra Gummelt's cluster (Gummelt, 1996). It consists of 33 atoms forming a circular figure (Fig. 5). One can prove that, owing to the atomic overlapping, these 33 atoms can be divided into only three groups of points that do not overlap each other and can consequently be decorated with different types of atoms.

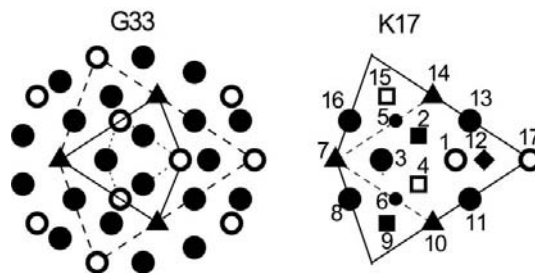


Figure 5

Gummelt's cluster G33 and the family of kite clusters. The K17 cluster is shown both inscribed in G33 (on the left site, dashed lines) and separately (on the right side). K7 and K4 are shown inscribed in G33, K7 the continuous line and K4 the dotted one. Atoms of different type (the non-overlapping ones) are marked with different symbols.

Another set of clusters, called kite clusters, have been introduced and thoroughly studied (Dąbrowska *et al.*, 2005). Consecutive members of this set are interrelated with each other by means of the inflation rules. The smallest cluster, K4, consists of four points divided into two independent groups. The next one, K7, consists of seven points (three independent groups) and the following one is K17 (Fig. 5), built of 17 points (seven independent groups). The entire infinite family of these clusters is described by Duda *et al.* (2007).

The kite clusters give an alternative method for the description of the Penrose tiling. Because of the overlapping rules the structure they form is more rigid. However, this rigidity enforces the local five-dimensional symmetry and reduces the number of optimized parameters during the refinement process. Furthermore, the relative number of atoms belonging to different groups of cluster's atoms is comparable with the chemical composition of real quasicrystals. They are, then, a good starting point for a refinement procedure.

The procedure for the structure-factor derivation is analogous to the one presented in the context of the Penrose tiling rhombic model. It proceeds as follows:

(i) We set a reference point within the boundaries of a cluster. Then, we establish the area of the atomic surface that would represent the distribution of the reference point. As in the case of the rhombic model, again the area is triangular.

(ii) The area found is projected onto the physical space. As a result, we obtain an AUC for clusters directed at a specific direction.

(iii) Filling the cluster with atoms takes place as in the rhombic model. The distance between the coordinates of an atom and the reference point is equal to the distance of this atom's distribution within the Penrose tiling and the distribution of the reference points.

(iv) The first difference, when compared with the rhombic model, occurs when one needs to take the overlapping areas into consideration. Since the overall probability distribution for the Penrose tiling is flat, the overlapping areas need to be merged and their level must be reduced to the constant intensity. After merging all the overlapping atoms, we obtain disjoint areas of non-overlapping atoms. They can be of

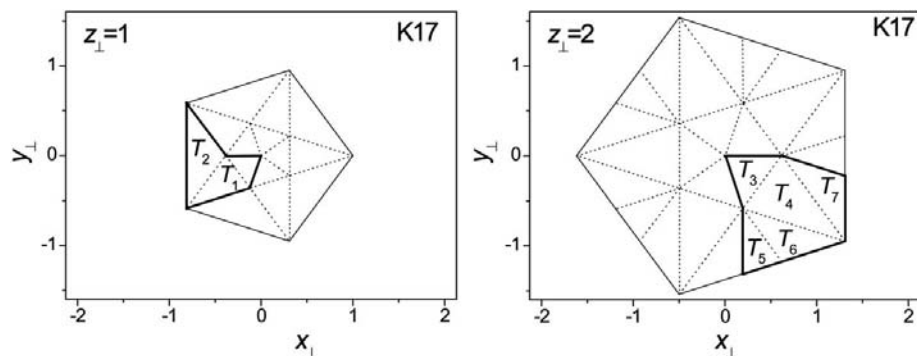


Figure 6
The division of the Penrose tiling's atomic surface into regions representing seven types of non-overlapping atoms decorating the K17 cluster: T_1 , atoms No. 1, 17; T_2 , 5, 6; T_3 , 7, 10, 14; T_4 , 3, 8, 11, 13, 16; T_5 , 12; T_6 , 2, 9; T_7 , 4, 15.

different types. The final division of the atomic surface for the K17 cluster is shown in Fig. 6.

(v) The sum of the Fourier transforms for all these areas leads to the structure factor for the cluster model of the Penrose tiling. The resulting formula is as follows:

$$F(\chi_x, \chi_y) = \text{re} \left\{ \sum_{t=1}^{t_{\max}} \sum_{j=1}^2 \exp(i\varphi_j) \times \sum_{\alpha=0}^4 \iint_{T_{t,j,\alpha}} \exp[i(\chi_x u_x + \chi_y u_y)] du_x du_y \right\}, \quad (29)$$

where $\varphi_j = j\varphi_0$, t_{\max} is the number of independent areas and in the case of cluster K17 it is equal to 7, and $T_{t,j,\alpha}$ is a triangular area number t of orientation α and lying on a pentagon for which $j = z_{\perp}$. The remaining symbols are as in equations (21)–(24).

(vi) The structure refinement involves establishing the types of atoms which decorate the areas, the occupation probability and the Debye–Waller factor.

While modeling the quasiperiodic structure, we can take into account both the cluster and the rhombic models. The rigidity of the first one can be of significant advantage during the initial part of the refinement. Only after the R factor is reduced to a level of 10% and lower can the atomic positions be released and refined as in the rhombic model. Following this procedure we obtained the resulting 8% R factor for the Al–Ni–Co alloy which was described above.

5. Conclusions

The applications of the average unit cell approach demonstrated in this paper are only the most essential ones and do not encompass the entire usability of the method. In this paper we limited the calculations to those which are needed to prove the AUC as an equivalent method to the multidimensional one. In the case of a perfect structure both methods lead to analogous results.

The AUC approach is nonetheless more flexible than the multidimensional method. Firstly, this is so since the AUC can be applied to the refinement of any type of structure, not only

quasicrystals but also, for instance, periodic crystals, modulated structures (Urban & Wolny, 2006), disordered structures (Orzechowski & Wolny, 2007) or structures for which the diffraction peak intensities scale fractally (Wolny *et al.*, 2000). The flexibility stems from the AUC's ability to work with the probability distributions of the physical atomic positions. Secondly, the interpretation of the parameters is much more intuitive under the AUC approach, as they all have a strict and clear physical meaning. Thirdly, the method allows the equation of a structure factor to be extended in a

manner identical to the one known from periodic crystals, and new parameters (for instance, the Debye–Waller factor or the shift from the initial position) immediately gain physical interpretation, while in order to incorporate new parameters in the multidimensional approach one needs to look for their multidimensional equivalents. Finally, under the AUC approach, taking atomic disorder into consideration comes with minimal burden for the method.

We obtained an analytical expression for the structure factor of freely decorated Penrose tiling using the average unit cell approach. Similar calculations for one-dimensional quasicrystals were presented by Wolny & Kozakowski (2003). The obtained formula (21) is very similar to the well known expression for periodic crystals. It consists of phase factors $[\exp(i\mathbf{k} \cdot \mathbf{r})]$ multiplied by the set of $T(k)$ values, which are the same for all possible decorations. This brings full parallelism between the structure factor for quasicrystals written in the physical space and the structure factor for periodic crystals.

The obtained formula makes use of only the physical atomic coordinates. This can then be easily extended, so that it could describe other physical properties of a structure that are accessible by the structure factor used to analyze periodic crystals.

The structure factor was tested on several differently decorated two-dimensional quasicrystals. Additionally, it was used to conduct the structure refinement of the Al–Ni–Co alloy. The resulting low value of the R factor proves the usefulness of the method.

APPENDIX A Oblique projection

The aim of this section is to derive a relationship between an AUC and an atomic surface. The relationship found will enable us to calculate theoretical coordinates of a probability distribution and prove the equations (16).

The starting point is an equation stating that for periodic crystals the dot product written between a reciprocal vector pointing to a diffraction peak and a position vector $\mathbf{K} \cdot \mathbf{R}$ must

be equal to a multiple of 2π . As $\mathbf{K} \cdot \mathbf{R}$ is a part of the complex exponent, 2π can be omitted and the resulting formula reads

$$\exp(i\mathbf{K} \cdot \mathbf{r}) = \exp[i(\mathbf{k}_\perp \cdot \mathbf{r}_\perp + \mathbf{k}_\parallel \cdot \mathbf{r}_\parallel)] = 1. \quad (30)$$

The exponent can be rewritten as

$$n_x(k_x u_x + k_{\perp x} x_\perp + k_{\perp z} z_\perp) + n_y(k_y u_y + k_{\perp y} y_\perp) + m_x(q_x v_x + q_{\perp x} x_\perp + q_{\perp z} z_\perp) + m_y(q_y v_y + q_{\perp y} y_\perp) = 0. \quad (31)$$

The last equation must be satisfied for any values of indexes n_x, n_y, m_x, m_y . This is possible only if

$$\begin{aligned} k_x u_x + k_{\perp x} x_\perp + k_{\perp z} z_\perp &= 0, \\ k_y u_y + k_{\perp y} y_\perp &= 0, \\ q_x v_x + q_{\perp x} x_\perp + q_{\perp z} z_\perp &= 0, \\ q_y v_y + q_{\perp y} y_\perp &= 0. \end{aligned} \quad (32)$$

Solving this system of equations with respect to u_x, u_y, v_x, v_y leads to

$$\begin{aligned} u_x &= -\frac{k_{\perp x}}{k_x} x_\perp - \frac{k_{\perp z}}{k_x} z_\perp, \\ u_y &= -\frac{k_{\perp y}}{k_y} y_\perp, \\ v_x &= -\frac{q_{\perp x}}{q_x} x_\perp - \frac{q_{\perp z}}{q_x} z_\perp, \\ v_y &= -\frac{q_{\perp y}}{q_y} y_\perp. \end{aligned} \quad (33)$$

We conclude:

(i) The formulas obtained relate the perpendicular coordinates of an atom with its position in an AUC. The transformation is linear, therefore we can interpret it as a projection of points of an atomic surface onto an AUC along directions given by ratios of appropriate coordinates of reciprocal basis vectors. Any distribution found within boundaries of an atomic surface, after a transformation, can be used as a probability distribution in an AUC approach. For instance, for the entire Penrose tiling, the AUC found numerically consists of four pentagons, the vertices of which are related to the atomic surface by the relationships (33).

(ii) The atomic surface of a Penrose tiling is regular. The corresponding AUC is usually not. This is so because the ratios $k_{\perp x}/k_x$ and $k_{\perp y}/k_y$ are not equal.

(iii) The relationships $v_x(u_x)$ and $v_y(u_y)$ can be found by eliminating x_\perp in the first and third equations and y_\perp in the second and fourth ones. The resulting formulas are

$$\begin{aligned} v_y &= \frac{q_{\perp y}}{q_y} \cdot \frac{k_y}{k_{\perp y}} u_y = -\tau^2 u_y, \\ v_x &= \frac{q_{\perp x}}{q_x} \cdot \frac{k_x}{k_{\perp x}} u_x + \left(\frac{q_{\perp x}}{q_x} \frac{k_x}{k_{\perp x}} \frac{k_{\perp z}}{k_x} - \frac{q_{\perp z}}{q_x} \right) z_\perp \\ &= -\tau^2 u_x - \left(\tau^2 \frac{k_{\perp z}}{k_x} - \frac{q_{\perp z}}{q_x} \right) z_\perp. \end{aligned} \quad (34)$$

The proof for ratios $(q_\perp/k_\perp)(k/q)$ being equal to $-\tau^2$ is easy although lengthy; it will therefore be omitted. To prove this,

Table 1

The coordinates of triangular areas of the Penrose tiling's atomic surface which describe the distribution of the chosen thick and thin rhombi.

These rhombi are shown in Fig. 1.

| Thick rhombus | | Thin rhombus | |
|--|------------------|---------------|---------------|
| $z_\perp = 1$ | | $z_\perp = 1$ | |
| $x_{\perp L}$ | $y_{\perp L}$ | $x_{\perp S}$ | $y_{\perp S}$ |
| $2\tau c_1$ | 0 | c_1 | s_1 |
| $-(\tau + 1)c_1$ | $(\tau - 1)s_1$ | $2\tau c_1$ | 0 |
| $-(\tau + 1)c_1$ | $-(\tau - 1)s_1$ | c_1 | $-s_1$ |
| $c_1 = \cos(2\pi/5); s_1 = \sin(2\pi/5)$ | | | |

one needs to find a general relationship among five-dimensional indexes when the physical coordinates are extended τ times. This relationship applied to the perpendicular coordinates would shorten them τ times. The set of basis vectors chosen for the AUC approach can illustrate this relationship. When the exact values of their coordinates are used, equations (34) read

$$\begin{aligned} u_x &= -x_\perp + 2z_\perp, & u_y &= \frac{1}{\tau^3} y_\perp, \\ v_x &= \tau^2 x_\perp - \tau \cdot z_\perp, & v_y &= -\frac{1}{\tau} y_\perp. \end{aligned}$$

The discussed relationship (16) becomes apparent.

(iv) Equations (34) give reason for introducing parameters u_{x0} and v_{x0} . Areas projected along x directions are not only linearly transformed but are also shifted ($u_{x0} = -z_\perp k_{\perp z}/k_x$ and $u_{x0} = -z_\perp q_{\perp z}/q_x$). To keep the relationship $v_x = -\tau^2 u_x$ valid, we need to add a phase factor as was done in the equation for every pentagon [equation (19)].

APPENDIX B

The shape of the probability distribution

The shape of the probability distribution used in an AUC approach can always be found numerically. In the case of perfect quasicrystals, however, thanks to the relationship between an AUC and an atomic surface, we can find such distributions in a strict way. For instance, if we want to find a distribution which describes the positions of atoms belonging to a thick rhombus presented in Fig. 1 then, in the first step, we need to establish five-dimensional indices of all vertices of such a rhombus. In this case they are: $\mathbf{A} = [0, 0, 0, 0, 0]$, $\mathbf{A}_1 = [0, 1, 0, 0, 0]$, $\mathbf{A}_2 = [0, 0, 1, 0, 0]$ and $\mathbf{A}_3 = [0, 1, 1, 0, 0]$. Then, we need to find the part of an atomic surface for which all four points A, A_1, A_2, A_3 are within the boundaries of an atomic surface. To achieve this we have to establish the perpendicular ($\Delta x_\perp, \Delta y_\perp, \Delta z_\perp$) coordinates of relative distances between these points. In this situation, they are: $\mathbf{w}_1 = \mathbf{A}_1 \mathbf{A} = [0.5(\tau - 1), 0.5(\tau + 2)^{1/2}, 1]$, $\mathbf{w}_2 = \mathbf{A}_2 \mathbf{A} = [0.5(\tau - 1), -0.5(\tau + 2)^{1/2}, 1]$, $\mathbf{w}_3 = \mathbf{A}_3 \mathbf{A} = [(\tau - 1), 0, 2]$. These vectors are used to cut out the appropriate part of the atomic surface. The process is presented in Fig. 2. The resulting area is triangular. We obtain similar results for a thin rhombus. The coordinates of the

obtained areas for both thick and thin rhombi are given in Table 1.

These areas projected onto physical space (or simply rescaled) form an average unit cell for the structural units of the Penrose tiling.

APPENDIX C

Fourier transform of a triangular distribution

The derivation of the structure factor involves computing a Fourier transform of a triangular probability distribution of a constant probability density. Let us assign numbers $p = 1, 2$ and 3 to the consecutive vertices of a triangle.

For a particular rhombus and a particular α , we can rewrite equation (24) as

$$T(\mathbf{k}) = \iint_{\Delta} \exp[i(\chi_x u_x + \chi_y u_y)] du_x du_y, \quad (35)$$

where φ_0 as a constant value is omitted here.

If we denote a particular vertex by the index 'p' (i.e. the coordinates are u_{px} and u_{py}) and the linear coefficient of the line connecting vertices l and m as a_{lm} then the resulting formula for the Fourier transform is

$$T(\mathbf{k}) = \frac{1}{\chi_y} [D_{12}(E_2 - E_1) + D_{23}(E_3 - E_2) + D_{31}(E_1 - E_3)], \quad (36)$$

where

$$D_{lm} = \frac{1}{\chi_x + \chi_y a_{lm}}, \quad E_p = \exp[i(\chi_x u_{px} + \chi_y u_{py})].$$

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