Bulk Termination of the Quasicrystalline Five-Fold Surface of Al$_{70}$Pd$_{21}$Mn$_9$

Z. Papadopolos* and G. Kasner
Institut für Theoretische Physik, Universität Magdeburg, PSF 4120, D-39016 Magdeburg, Germany

J. Ledieu and E.J. Cox
Surface Science Research Centre, The University of Liverpool, Liverpool L69 3BX, UK

N.V. Richardson and Q. Chen
Department of Chemistry, University of St. Andrews, Fife, Scotland

R.D. Diehl
Department of Physics, Pennsylvania State University, University Park, PA 16802, USA

T.A. Lograsso and A.R. Ross
Ames Laboratory, Iowa State University, Ames, IA 50011, USA

R. McGrath
Surface Science Research Centre and Department of Physics, The University of Liverpool, Liverpool L69 3BX, UK

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The structure of the Al$_{70}$Pd$_{21}$Mn$_9$ surface has been investigated using high resolution scanning tunnelling microscopy (STM). From two large five-fold terraces on the surface in a short decorated Fibonacci sequence, atomically resolved surface images have been obtained. One of these terraces carries a rare local configuration in a form of a ring. The location of the corresponding sequence of terminations in the bulk model $M$ of icosahedral $i$-AlPdMn based on the three-dimensional tiling $T^{(2F)}$ of an F-phase has been estimated using this ring configuration and the requirement from the LEED work of Gierer et al. that the average atomic density of the terminations is 0.136 atoms per $\text{Å}^2$. A termination contains two atomic plane layers separated by a vertical distance of 0.48 Å. The position of the bulk terminations is fixed within the layers of Bergman polytopes in the model $M$: they are 4.08 Å in the direction of the bulk from a surface of the most dense Bergman layers. From the coding windows of the top planes in terminations in $M$ we conclude that a Penrose (P1) tiling is possible on almost all five-fold terraces. The shortest edge of the tiling P1, is either 4.8 Å or 7.8 Å.

The experimentally derived tiling of the surface with the ring configuration has an edge-length of 8.0 ± 0.3 Å and hence matches the minimal edge-length expected from the model.

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I. INTRODUCTION

More than ten years ago, the discovery that centimetre size samples of decagonal $d$-AlCuCo and icosahedral $i$-AlPdMn could be grown opened up the possibility of surface studies of these quasicrystals. Since then other quasicrystal samples have been grown to similar dimensions. To date, most surface studies have been performed on the five-fold surface of $i$-AlPdMn. A consensus has emerged from these studies that this surface, after fairly standard ultra-high-vacuum (UHV) sputtering and annealing procedures, is itself quasicrystalline. In this work, using a combined experimental and theoretical approach, we show that this surface can be considered to be a termination of the known bulk structure.

The dynamical low-energy electron diffraction (LEED) analysis carried out by Gierer et al. indicated that the five-fold surface of the $i$-AlPdMn quasicrystal retained the bulk quasicrystallinity. X-ray photoelectron diffraction (XPD) studies are also consistent with a quasicrystalline surface nature. Large flat terraces may be produced, and scanning tunnelling microscopy (STM) studies have presented similar images of the quasicrystalline surface. Schaub et al. produced detailed STM images of the terraces that reveal a dense distribution of dark pentagonal holes of edge-length circa 4.8 Å oriented parallel to each other, together with a more random distribution of bright protrusions. They correlated measurements of structural elements both within the terraces and across steps on the surface.

Later, we demonstrated a correspondence of these measurements with the geometric model $M$ for atomic positions of an F-phase. The model $M$ is based on the three-dimensional icosahedral tiling $T^{(2F)}$ decorated essentially by Bergman/Mackay polytopes.
observed terrace structure of the surface was explained in terms of the layer structure of the bulk model. The dark pentagons observed on the surface corresponded to the Bergman polytopes \( \text{P1} \) in the bulk layers. The position of a given type of terrace was matched to a layer characterized by a density of certain Bergman polytopes and their distribution pattern. We assumed that the surface termination respects the integrity of the Bergman polytopes as clusters, at least in the most dense layers, and we supposed that such a layer of Bergman polytopes is exactly below the termination. However, under these assumptions it was not possible to explain the observed edge-length (circa 4.8 Å) of the dark pentagonal holes, as this was bigger by the factor \( \tau = (\sqrt{5} + 1)/2 \) than the pentagonal surfaces of the Bergman polytope (circa 3 Å) [19,20,21].

Later Shen et al., using an autocorrelation analysis showed that the surface structure is consistent with a bulk structure based on truncated pseudo-Mackay icosahedra and (therefore) Bergman clusters. A further test of this limit of those previous STM studies (Refs [22–24]), was that the resolution of the images, while subnanometre, was not atomic. Therefore direct comparison with bulk models was not straightforward. Additionally, the presence of bright protrusions disrupted any attempted tiling, and so comparison with tiling models was not possible. In a previous paper, we reported an improved sample preparation technique. This led to a more perfect surface devoid of protrusions (section II), and this in turn led to improved resolution in the STM images. The better resolution, together with the structural perfection, allowed us to demonstrate that the surface structure is consistent with a bulk termination \( \text{P1} \), using the bulk model of Boudard et al. [25].

In this paper we try to find the position of terminations in the bulk model \( \mathcal{M} \) demanding (i) that the terminations are ordered in a decorated Fibonacci sequence (sections II A, II C), as in Refs [26–28], and (ii) that the average density of terminations is 0.136 atoms per Å\(^2\), as determined by Gierer et al. [21] (section II D). The atomically resolved images of the surface that allow us to map the local patterns of the STM images (sections II, IV A) to the local atomic configurations in the terminations in \( \mathcal{M} \) (section IV A), also prove our Ansatz from section II D which fixes the position of the bulk termination to be 4.08 Å deeper within the layer of Bergman polytopes than we expected in Refs [26–28]. With this new position of the termination, the edge-length of the dark pentagonal holes observed by Schaub et al. [14] is now understood (section IV A). Moreover we conclude that the terminations in the bulk model \( \mathcal{M} \) (section IV A), also prove our Ansatz from section II D. The edge-length of the dark pentagonal holes, observed by Schaub et al. [14], is now understood. The pentagonal surfaces of the Bergman polytopes (circa 4.08 Å) were constructed in Refs [17,18,20,21]. For details on Bergman and Mackay polytopes, see Ref 19. The geometric model is based on the Katz-Gratias model [22,23] that is explained by Elser in a three-dimensional “parallel space”, \( \mathbb{E}_p \), the space in which the model projected from \( \mathbb{D}_6 \) lattice [21,22] exists. The atoms of \( \text{i-AlPdMn} \) or \( \text{-AlCuFe} \) can be placed on three translational classes of atomic positions with respect to the \( \mathbb{D}_6 \) lattice, and are denoted by \( \mathbb{D}_6(q, \varphi) \), and \( \mathbb{D}_6(q, \varphi, \alpha) \). These atomic positions in \( \mathbb{E}_p \) are coded by the corresponding “windows” or “acceptance domains” in the three-dimensional “perpendicular space”, \( \mathbb{E}_l \). Note that the six-dimensional \( \mathbb{D}_6 \) lattice, which models an \( \text{F}- \) phase, acts in the six-dimensional space that is a sum of \( \mathbb{E}_l \) and \( \mathbb{E}_p \). These windows in \( \mathbb{E}_l \) are denoted by \( W_0 \), \( W_1 \), and \( W_2 \), respectively. The windows of the model \( \mathcal{M} \) were constructed in Refs [24,25]. The tiling \( \tau T^{(2F)} \) defines the quasiperiodic structure. More accurately, the model \( \mathcal{M} \) is supported by \( \tau T^{(2F)} \), the tiling \( \tau T^{(2F)} \) scaled by the factor \( \tau = (\sqrt{5} + 1)/2 \). The quasilattice points of \( \tau T^{(2F)} \) are in the class of \( q \in D_6 \).

All points of the quasilattice which contains the vertices of the tiling \( \tau T^{(2F)} \) can be embedded in a sequence of planes orthogonal to the five-fold symmetry axis of an icosahedron (“five-fold direction”). The planes orthogonal to the axis are the “five-fold planes”. The planes appear in a sequence and have been classified (by particular coding regions in the window \( W_{7+2F} \)) into five types, \( \pm 1, \pm 2, \pm 3, \pm 4, \pm 5 \), see Ref 21. The planes of type 1 to 4 are ordered in the Fibonacci sequence with intervals \( m \) and \( l \). If the planes of type 5 are included, the sequence of planes forms a “decorated Fibonacci sequence” with separations \( s \) (short), \( m \) (medium), \( l \) (long), where \( l = \tau m = \tau^2 s \), see Fig 13 in section IV A. How is the decorated Fibonacci sequence defined? Let us consider the Fibonacci sequence of intervals \( M = l \) and \( L = \tau l \). If we rename \( M \) by \( l \) and “decorate” the interval \( L \) by two points, such that \( L = m \cup s \cup m \), the decorated Fi-
bonacci sequence appears. For \(i\)-AlPdMn that has the standard distance parallel to the five-fold direction is \(\tau = 4.56\ \text{Å}\), and is modeled by \(\tau T^\ast(2F), s = \frac{2}{\tau + 2}\) \(\tau = 2.52\ \text{Å}, m = \tau \left(\frac{2}{\tau + 2}\right) = 4.08\ \text{Å}, l = \tau^2 \left(\frac{2}{\tau + 2}\right) = 6.00\ \text{Å}.

In the planes of type 1 a quasiperiodic tiling \(T^\ast(A1)\) appears scaled by a factor \(\tau\). In the planes of type 2, 3 and 4, fragments of the same tiling of a plane by golden triangles appear (see Ref. [4], Fig. 7), with the same inflation properties as in the tiling \(T^\ast(A1)\).

In Ref. [4], the model is compared to the ideal icosahedral monograin under the assumption that the terraces on the surface of the material are like the planes in the bulk, i.e. not reconstructed. This we will first assume and then support in this paper. The terraces observed by Schaub et al. [4] were related to the sequence of the planes of the model \(\mathcal{M}\) described above, see also Ref. [3]. Whereas Schaub et al., after annealing at \(\approx 800^\circ\text{C}\) observed only Fibonacci ordered step heights \(m\) and \(l\) on the surface, Shen et al., after annealing at \(\approx 630^\circ\text{C}\) also detected the step height \(s\), see Ref. [4].

In this paper we study the fine structure (local atomic configurations) within the observed terraces and compare it to the geometric model \(\mathcal{M}\). Whereas in Ref. [3] we succeeded in relating the sequence of the terrace-like five-fold surfaces of Schaub et al. to the layers of the Bergman polytopes in the geometric model \(\mathcal{M}\), in this paper, using high resolution STM images of a five-fold surface we will fix the position of the planes within the layers of Bergman polytopes.

In order to recognize and identify the fine structure of the observed surface, we consider certain tilings in the five-fold planes and a covering with a set of prototiles among which are the pentagons and pentagonal stars. These tilings will be locally derived from the tiling \(T^\ast(A1)\). The local derivation will be exact to a certain stage, and thereafter, random. The tiling \(T^\ast(A1)\) scaled by the factor \(\tau\) defines the quasiperiodic structure of the planes on the surfaces according to the model \(\mathcal{M}\) introduced above. The prototiles in the tiling \(T^\ast(A1)\) are golden triangles. The edges of the triangles in the tiling are parallel to the two-fold symmetry axes of an icosahedron (“two-fold directions”) and are of two lengths, \(2\) and \(\tau 2\). The three-dimensional model \(\mathcal{M}\) is supported by the tiling \(\tau T^\ast(2F)\) and consequently in the five-fold surfaces by \(\tau T^\ast(A1)\). Hence the edges are \(\tau 2\) and \(\tau^2 2\). With the standard value \(2 = 4.795\ \text{Å}\) in the case of \(i\)-AlPdMn, \(\tau 2 = 7.758\ \text{Å}\) and \(\tau^2 2 = 12.553\ \text{Å}.

The structure on the surface observed by STM can be tiled uniquely only if the tiling, as an abstract structure, is derivable from the set of quasilattice points, and if the rules of the local derivation are defined on relatively small distances with respect to the area of the observed surface.

B. Tilings and Coverings with Pentagonal Prototiles contained in the Tiling \(T^\ast(A4)\)

As an intermediate step we locally derive the tiling \(T^\ast(z)\) with pentagon, acute rhombus and hexagon as prototiles from the quasilattice \(T^\ast(A4)\), as shown in Fig. 1. The tiling has an inflation factor \(\tau\). It is clear that the tiling \(T^\ast(z)\) can be reconstructed from its own quasilattice points. All edges of the prototiles in \(T^\ast(z)\) are of length \(\tau\ 2\). In the geometric model \(\mathcal{M}\) the prototiles are augmented by a factor \(\tau\), so the edge-length is \(\tau^2 2 = 12.553\ \text{Å}\). All prototiles of \(T^\ast(z)\) are the unions of golden triangles of the previous tiling \(T^\ast(A4)\), as shown in Fig. 1. If we keep that content, the window of the tiling is identical to the window of \(T^\ast(A4)\) (because none of the vertex (quasilattice) points is omitted). The coding window of the tiling \(T^\ast(z)\), without content of golden triangles, is shown in Fig. 2. Small fractions of the tiling \(T^\ast(z)\) have been observed in the five-fold surfaces of decagonal \((d)\)-AlCuCo.

FIG. 1: The tiling \(T^\ast(z)\) of the plane with the acute rhombus, pentagon and hexagon as the prototiles. The tiles are marked by thick lines and different gray shadows. The tiling \(T^\ast(A4)\), from which \(T^\ast(z)\) is locally derived, is shown in background using thin lines.

From the intermediate tiling \(T^\ast(z)\) we can locally derive a covering of the tiling \(T^\ast(A4)\). This covering is by two cells in the shape of pentagons, the smaller one, \(D^a\), of edge-length \(2\) and the bigger, \(D^b\), of edge-length \(\tau 2\), as shown in Fig. 3(a). Let us denote this covering of the tiling \(T^\ast(A4)\) by \(C^A_{T^\ast(A4)}\). Each acute rhombus from \(T^\ast(z)\) is transformed into a pair of pentagons of edge-length \(2\) (shown in the left-hand side of Fig. 3(a)), and each hexagon is transformed into a pair of overlapping pentagons of edge-length \(\tau 2\) (right-hand side of Fig. 3(a)). The remainder of the tiling \(T^\ast(A4)\) should be covered by pentagons of edge-length \(\tau 2\) as in the tiling \(T^\ast(z)\), see Fig. 1. The above-defined covering \(C^A_{T^\ast(A4)}\) of the tiling \(T^\ast(A4)\) is a sub-covering of the covering of Kramer, \(C^k\). Kramer also covers the tiling \(T^\ast(A4)\) by two pentagons of the same size as above. These cells are projected De lone cells \(D^a\) and \(D^b\) of the lattice \(A_4\) in \(E_4\). In \(E_4\) they are denoted by \(D^a_{\parallel}\) and \(D^b_{\parallel}\) respectively. Let us denote Kramer’s covering by the symbol \(C^k_{T^\ast(A4)}\). The set
of pentagons in \( C^{*}_{\tau(A_4)} \) of edge-length \( \tau(2) \) is identical to the set of \( D_\parallel \)'s in \( C^{k}_{\tau(A_4)} \). The set of pentagons in \( C^{k}_{\tau(A_4)} \) of edge-length \( 2 \), derived from the acute rhombuses, is a subset of the set of all \( D_\parallel \)'s in \( C^{k}_{\tau(A_4)} \), and therefore the covering \( C^{k}_{\tau(A_4)} \) of \( \tau(A_4) \) is a subcovering of the covering \( C^{k}_{\tau(A_4)} \). Whereas the thickness of the covering of \( C^{k}_{\tau(A_4)} \) is \( C^{k} = 3 - \tau \approx 1.382 \), the thickness of the covering of the sub-covering \( C^{k}_{\tau(A_4)} \) is \( C^{*} = 2\tau - 2 \approx 1.236 < 1.382 \). (For an explanation of the thickness of the covering see Ref. \[32\]. As a reference: a thickness of the covering of a space by a tiling always equals 1.) In the sub-covering \( C^{*}_{\tau(A_4)} \) only the single and double decking (covering \[2\] of the tiles by the covering clusters are present. The triple decking, which exists in the covering \( C^{k}_{\tau(A_4)} \) is excluded in \( C^{*}_{\tau(A_4)} \). The window of the sub-covering \( C^{*}_{\tau(A_4)} \) of \( \tau(A_4) \) by two pentagons without the content of golden triangles is presented in Fig. \[4\].

![FIG. 3: (a) The derivation \( \mathcal{T}^{(z)} \rightarrow C^{*}_{\tau(A_4)} \) is in the top part of the figure; (b) \( \mathcal{T}^{(z)} \rightarrow \mathcal{T}^{(p1)} \) is in the bottom part of the figure.](image1)

From the tiling \( \mathcal{T}^{(z)} \) let us keep all acute rhombuses, and replace each hexagon by two overlapping pentagons (as in the sub-covering \( C^{*}_{\tau(A_4)} \)). This is an exact local derivation, shown in the left-hand side of Fig. \[3\](b). At this stage we randomly choose one of the pentagons from each overlapping pair, and the rest of each hexagon unites with the neighboring acute rhombus. In this way, either a crown or a pentagonal star appears to replace the rhombus, and we obtain a partly random tiling \( \mathcal{T}^{(p1)} \), see the right-hand side of the Fig. \[3\](b). The ideal class of tilings \( P1 \) with the inflation factor \( \tau \) are described in Refs. \[2\] and \[32\]. In Fig. \[3\](a), the window that exactly defines the quasilattice of the tiling \( \mathcal{T}^{(p1)} \) is inscribed in the window of the tiling \( \mathcal{T}^{(A_4)} \).

![FIG. 4: The window of the covering \( C^{*}_{\tau(A_4)} \) without the content of golden triangles, inscribed by the thick lines in the window of the tiling \( \mathcal{T}^{(A_4)} \).](image2)

There is another tiling of a plane by pentagonal stars, pentagons and obtuse rhombuses introduced by Niizeki. Let us call it the Niizeki star-tiling and denote it by \( \mathcal{T}^{(n)} \). The inflation factor of this tiling is also \( \tau \). In Fig. \[6\] we derive this tiling from the tiling \( \mathcal{T}^{(z)} \). In Fig. \[6\] (top part of Fig. \[6\]) on the left-hand side, from the set of all stars, only the locally derivable stars are presented. The locally derivable star appears whenever there exists an acute rhombus neighboring one or two hexagons, each by an edge. Between these stars, there appear obtuse rhombuses. In Fig. \[6\] on the right-hand side the white spaces around the isolated acute rhombuses are framed by thick lines. Inside these patches, there appear pairs of overlapping stars, inscribed in one single place in the figure and marked by an arrow. Their overlap is exactly the acute rhombus. Up to the choice of one star from each pair of overlapping stars, the local derivation of the tiling is exact. The exact tiling of the plane by the stars, obtuse rhombuses and pentagons, \( \mathcal{T}^{(n)} \), is uniquely determined by its window inscribed in the window of \( \mathcal{T}^{(A_4)} \), see Fig. \[6\]. It is the window of Niizeki tiling. We randomly choose a star from each overlapping pair of stars indicated in the bottom part of Fig. \[6\] and obtain a partly random tiling \( \mathcal{T}^{(n)} \).

![FIG. 5: (a) The window of \( \mathcal{T}^{(p1)} \) is inscribed in the window of \( \mathcal{T}^{(A_4)} \) by thick lines. (b) The exact tiling of the plane by the stars, obtuse rhombuses and pentagons, \( \mathcal{T}^{(n)} \), is uniquely determined by its window inscribed by thick lines in the window of \( \mathcal{T}^{(A_4)} \). It is the window that codes the Niizeki tiling \( \mathcal{T}^{(n)} \).](image3)

Both exact tilings, \( \mathcal{T}^{(p1)} \) and \( \mathcal{T}^{(n)} \), can be locally derived from their respective quasillattices points. In the reconstruction of tilings \( \mathcal{T}^{(p1)} \) and \( \mathcal{T}^{(n)} \) from the respective quasillattices there appear: (i) pairs of pentagonal sets of points centered in each other and mutually rotated by \( 2\pi/10 \). The set of points of the smaller size (the smallest pentagonal set in the tiling) is on the neighboring distances \( 2 \), the bigger, on neighboring distances \( \tau^2 \). Each pair leads to the pentagonal star; (ii) the isolated pentagonal sets with neighboring distances \( \tau \) are to be connected in pentagons. In order to reconstruct the tiling \( \mathcal{T}^{(p1)} \), it is enough to draw the pentagons from the isolated five-tuples of five-fold symmetrically ordered points. In order to reconstruct the tiling \( \mathcal{T}^{(n)} \) one draws the stars from the pairs of pentagonal sets defined above. One can show that in an abstract sense the tilings \( \mathcal{T}^{(p1)} \) and \( \mathcal{T}^{(n)} \) can be mapped one-to-one to each other. If we consider an experimental atomically resolved five-fold surface, and tile the observed surface, we first have to identify the surface by a plane in the model which we will call an \( \mathcal{M} \)-plane. Then we determine the coding window of the plane in \( \mathcal{E}_1 \), the \( \mathcal{M} \)-plane window, and we place the biggest possible window of an exact tilings \( \mathcal{T}^{(p1)} \) or \( \mathcal{T}^{(n)} \) in the \( \mathcal{M} \)-plane window, see Figs. \[3\] and \[4\]. Following these arguments, we will determine the edge-length of a possible tiling of an observed surface by the prototiles of the tiling \( P1 \) in section \[1\].
C. Atomic Positions in Five-Fold Planes of the Geometric Model \( M \)

In section II B we have derived the tilings \( T^*(z) \), \( T^*(p_1) \) and \( T^*(n) \) either from the ideal tiling \( T^*(A_4) \) or from their own corresponding quasilattices. We have been considering exclusively these points \( q \in D_6 \) that belong to the underlying tiling of the model, \( \tau^*T^*(A_4) \). Consequently the edge-lengths in both locally derived tilings, \( T^*(p_1) \) and \( T^*(n) \) were of length \( r^2g = 12.553\AA \). If we also take into account the decoration of the tiling by Bergman/Mackay polytopes, the window of the quasilattice points of type \( q \in D_6 \), \( W_{q|b} \) becomes the polytope derived in Ref. 15.

In order to study the five-fold planes of the model \( M \), we present two important general facts that we implicitly use in all our considerations.

(i) The reciprocal lattice of the root-lattice \( D_6 \) we denote by \( D_6^{*cc} \). The lattice \( D_6^{*cc} \) is also known as the weight-lattice \( D_6^{*w} \). If one icosahedrally projects \( D_6^{*cc} \) to the parallel space, \( E_{||}/(E_{||}^\perp) \), an icosahedral \( \mathbb{Z}(\tau) \)-module appears. The module points in a plane of a three dimensional (icosahedral) \( \mathbb{Z}(\tau) \)-module in \( E_{||} \), under the *-map, i.e., \( \tau \rightarrow -1/\tau \), are mapped in \( E_{||}^\perp \) into a plane too. The section of this plane in \( E_{||}^\perp \) through the three-dimensional window (acceptance region of the three-dimensional quasilattice) defines a two-dimensional window of the quasilattice in a corresponding plane in \( E_{||} \). The analogous statement holds true for the lines. These are the general properties of a \( \mathbb{Z}(\lambda) \) module with quadratic irrationality \( \lambda \). In our considerations \( \lambda = \tau = (\sqrt{5}+1)/2 \). The above statement is valid for the modules with symmetries such as icosahedral, five-fold, ten-fold, eight-fold and twelve-fold.

(ii) Let us consider the four translational classes with respect to the root-lattice \( D_6 \) of six-dimensional points \( \frac{1}{2}(n_1, \ldots, n_6) \in D_6^w \), where \( n_i \) are integers. The condition for an atomic position \( x = \frac{1}{2}(n_1, \ldots, n_6) \) to be in a five-fold plane in \( E_{||} \) or \( E_{||}^\perp \) is a class-function presented in Table 1. Hence the atomic positions in a five-fold plane of a \( D_6^{*w} \)-icosahedrally projected \( \mathbb{Z}(\tau) \)-module belong to the single class, \( q_{ab}(\equiv q) \), \( b \), \( a \) or \( c \).

Using the facts (i) and (ii), in the geometric model \( M \) we code each five-fold plane containing a class of atomic positions in \( E_{||} \) by the five-fold dissection in \( E_{||}^\perp \) of the single window \( W_q \), \( W_b \) or \( W_a \), corresponding to that class.

D. Densities of Five-Fold Planes and Terminations of Five-Fold Surfaces in the Geometric Model \( M \)

In the work of Gierer et al.\cite{4} an average density of “terminations” of five-fold surfaces has been determined to be \( \rho_{q+b} = \rho_q + \rho_b = 0.136 \) atoms per \( \AA^2 \). By the density of the termination the authors mean the sum of the densities of two atomic planes on a surface separated by a vertical distance of 0.48\AA, and consequently each “termination” corresponds to a pair of planes separated by this distance. Let us suppose that the surface (top) planes are of type \( q \), then the planes 0.48 \AA below, in the geometric model \( M \), are of type \( b \). Let us calculate \( \rho_{q+b}(z_\parallel) \) in the model, where \( z_\parallel \) is along a five-fold axis orthogonal to surfaces on the surface, and let us plot this value along the corresponding \( z_\perp \), \( \rho_{q+b}(z_\perp) \). The result is shown in Fig. 7.

![FIG. 6: Local derivation: \( T^*(z) \rightarrow T^*(n) \). In the text, the top part of the Figure is referred to as (a) and the bottom part as (b).](image)

TABLE I: The condition for atomic positions \( x = \frac{1}{2}(n_1, \ldots, n_6) \) to be in a five-fold plane in \( E_{||} \) or \( E_{||}^\perp \) is a class-function. The symbols \( e \) and \( o \) stand for even and odd integers, respectively. The symbol \( n^0_6 \) is a unit normal to the five-fold plane in \( E_{||} \) or \( E_{||}^\perp \), respectively, \( x_1 \in E_{||} \) and \( x_2 \in E_{||}^\perp \), where \( x \) is the point in six-dimensional space, \( E_{||} + E_{||}^\perp \). The scalar product is given in the units \( [\kappa] \), \( \kappa = 1/([\sqrt{2} (\pi + 2)] \).

| class-criterion | class | \( n^0_6 \cdot x_{||}[\kappa] \) | \( n^0_6 \cdot x_{||}[\kappa] \) |
|-----------------|------|-----------------|-----------------|
| \( \frac{3}{2}(e_1, \ldots, e_6) \); \( \frac{3}{2} \sum e_i \) = even | \( q_{o|b} \) | \( e + \epsilon \tau \) | \( e + \epsilon \tau \) |
| \( \frac{3}{2}(e_1, \ldots, e_6) \); \( \frac{3}{2} \sum e_i \) = odd | \( b \) | \( e + \epsilon \tau \) | \( e + \epsilon \tau \) |
| \( \frac{3}{2}(o_1, \ldots, o_6) \); \( \frac{3}{2} \sum o_i \) = odd | \( a \) | \( o + \epsilon \tau \) | \( o + \epsilon \tau \) |
| \( \frac{3}{2}(o_1, \ldots, o_6) \); \( \frac{3}{2} \sum o_i \) = even | \( c \) | \( o + \epsilon \tau \) | \( o + \epsilon \tau \) |

![FIG. 7: Density \( \rho_{q+b} \) of the pairs of five-fold planes in bulk model \( M \): a q-plane and a b-plane, 0.48\AA below the q-plane \( \rho_{q+b} \) as a function of \( z_\parallel \) in units of \( r^2g \). The images of z-axes in \( E_{||} \), \( z_\parallel \), is chosen such that \( z_\parallel \) points into opposite direction of the bulk. \( \rho_{q}(z_\parallel) \) is the density of a q-plane, \( \rho_{b}(z_\parallel) \) is the density of a b-plane shifted by \( c^\perp_{\parallel-b} = [r^2g/(\pi + 2)] \). In the figure the old and the new coding regions of the (decorated) Fibonacci sequence of planes that represent the surface terraces in \( M \) are marked. In the new region, the representative plane of the biggest clear terrace of Schauli\cite{3} is marked by S8 on a new position. The condition for appearance of the Ring-plane in a sequence mll (R)ml is determined and a representative of a Ring-plane (R) together with a representative of the following Clear-plane (C) are marked. Finally the region of existence for P1 tilings on a q-plane is denoted and particular minimal edges are attached to their coding regions, see section IV.](image)

The function \( \rho_{q+b}(z_\parallel) \) has clear (almost flat) plateau. The appearance of the plateau is due to the polytopal shape of the coding windows \( W_q \) and \( W_b \) in the geometric model \( M \). In particular the window \( W_q \), that defines the surface (top) plane in a termination, differs strongly from the spherical shape. The plateau of

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the function $p_{q+b}(z_\perp)$ simultaneously contains the maxima of the function and has a value that approximately equals the average density of terminations determined by Gierer et al.\cite{Gierer1992}, which is 0.136 atoms per Å². It is easy to conclude that all terminations on terraces must have equal densities. Consequently an interval on $z_\perp$ under the plateau (the “carrier” of the plateau) codes the terminations and indicates the new coding of surface $q$-planes to be shifted from the old value that we expected in Ref.\cite{Schaub1992}. In those papers\cite{Schaub1992,Schaub1993}, we supposed that a single surface $q$-plane has to have the highest density. In accordance with this Ansatz, at least some of the dense layers of Bergman polytopes were below the surfaces. But the dark pentagons observed by Schaub\cite{Schaub1992}, that we put in correspondence to the Bergman polytopes in the layer below the surface, were bigger by a factor $\tau$ than the faces of Bergman polytopes\cite{Schaub1993}. Let us shift the surfaces of terraces by 4.08 Å in the direction of the bulk (-4.08Å along $z_\parallel$) in “parallel” (observable) space, such that the $q$-plane on a terrace dissects the Bergman polytopes of the layer and the section of each Bergman polytope is a pentagon of edge-length 4.8Å, approximately the size of the dark pentagons observed by Schaub\cite{Schaub1992}. This shift in $E_\parallel$ corresponds to the shift by $[2\tau/(\tau + 2)]\otimes$ along $z_\perp$ in orthogonal space. Indeed, the coding interval of $q$-planes that forces the planes on the surface to appear in a Fibonacci sequence (or in a decorated Fibonacci sequence) is placed under the plateau of the function $p_{q+b}(z_\perp)$ by this shift, see Fig.\cite{Schaub1992}. We suppose that the terrace-like five-fold terminations do appear in a Fibonacci (or decorated Fibonacci) sequence such that the top $q$-planes in terminations need not be the most dense among the $q$-planes, but the above defined “terminations”, the pairs of planes on a surface, have the highest densities among all such pairs of $q$- and $b$-planes in the geometric model $\mathcal{M}$. We check our hypothesis (Ansatz) on two large terraces in section III.

III. FIVE-FOLD SURFACES IMAGED BY STM; SURFACE PREPARATION AND STM RESOLUTION

In this section we describe the surface preparation we have developed to obtain large flat terraces and low surface corrugation in STM experiments. We contrast STM results using our optimum preparation with results previously published by us and other groups\cite{Giersch1992,Schaub1992,Schaub1993}.

Fig.\cite{Giersch1992} shows data from the surface of $i$-Al-Pd-Mn after the two different preparation procedures. In each case the quasicrystal samples were grown at Ames Laboratory using the Bridgman method\cite{Giersch1992}. After being cut perpendicular to their five-fold symmetry axes in air, the sample surfaces were prepared\cite{Giersch1992} by polishing. For the first preparation, Preparation I, the sample was polished using 6, and 1 μm diamond paste for one hour. In-vacuum preparation consisted of a few cycles of argon ion sputtering at 1 keV energy and a normal incidence angle followed by annealing for periods of about 1 hour at 970 K. The results are shown in Fig.\cite{Giersch1992}(left hand panels (a) and (c)). For the second preparation, Preparation II, a further polish using 0.25 μm diamond paste was used. The surface was prepared in-vacuum by several cycles of sputtering with 0.5 keV Ar ions, with a sputtering angle of 20°-30° relative to the surface parallel, followed by annealing to 970 K for two hours (in total twelve hours of annealing); Fig.\cite{Giersch1992}(right hand panels (b) and (d)) show the results.

When large scale scans are compared (Fig.\cite{Giersch1992}(a) and (b)), it is evident that larger terraces are obtained using Preparation II. For Preparation I, the largest terraces are of the order of 1200 Å in magnitude. For Preparation II terraces of width 4000 Å and length of micron size were obtained. Further differences between the results of the preparation techniques are observed when scans of smaller area are compared. Fig.\cite{Giersch1992}(c) and (d) show 100 Å × 100 Å areas of each surface. Clearly the surface in Fig.\cite{Giersch1992}(c) is not as well resolved as that in Fig.\cite{Giersch1992}(d); the bright spots in Fig.\cite{Giersch1992}(c) correspond to protrusions of height up to 2.0 Å, while dark spots are associated with holes of depth estimated to be at least 1.5 Å. This STM image is comparable to those in the work of Schaub et al.\cite{Schaub1992,Schaub1993}. This can be contrasted with the surface shown in Fig.\cite{Giersch1992}(d) where there are no large protrusions and the surface corrugation within the terraces is $< 1$ Å. Because the STM tip can scan the surface more closely, features on the surface are better resolved. The features in this image have dimensions typical of atomic sizes (2-3 Å). Larger features (4-6 Å) are also evident and probably represent groups of a few atoms. The LEED patterns from each of these surfaces are qualitatively identical, but the range of electron beam energies over which the LEED patterns are obtained is much larger (10-300 eV) using Preparation II than for Preparation I (40-180 eV).

The LEED patterns have very sharp diffraction spots, a low background, and show five-fold symmetry.

FIG. 8: (a) 1500 Å × 1500 Å STM image showing atomically flat terraces from a surface prepared using Preparation I. (b) 17500 Å × 17500 Å STM image showing atomically flat terraces from a surface prepared using Preparation II. (c) 100 Å × 100 Å STM image of a flat terrace that we call the “Clear”, C-terrace from a surface prepared using Preparation I (bias voltage 2.29 V, tip current 0.59 nA). (d) 100 Å × 100 Å high resolution STM image of the same C-terrace obtained on the five-fold surface using Preparation II (V=1 V, I= 0.3 nA).

The resolution can be put on a semi-quantitative basis by calculating the two-dimensional lateral autocorrelation functions of the images of Fig.\cite{Giersch1992}(c) and (d). These are shown in Fig.\cite{Giersch1992}(a) and (b) respectively. While the symmetry of both autocorrelation patterns is similar, the pattern of Fig.\cite{Giersch1992}(b) is considerably clearer and the correlation maxima extend to longer distances indicating a
higher degree of quasiperiodic order.

For a more quantitative comparison a radial distribution function (RDF) has been calculated in both cases. The procedure consists of dividing the 360° around the centre of the autocorrelation function in increments. Along each line corresponding to each increment, the distances from the centre to the maxima are measured. All the measurements are then averaged and plotted as histograms (Fig. 8(c) and (d)). It can be seen that there is considerably more structure in the RDF in Fig. 8(d) than in that of Fig. 8(c).

FIG. 9: (a) 100 Å × 100 Å lateral autocorrelation function of the STM image of Fig. 8(c). (b) 100 Å × 100 Å lateral autocorrelation function of the STM image of Fig. 8(d). (c) Radial distribution function calculated from the autocorrelation pattern of (a). (d) Radial distribution function calculated from the autocorrelation pattern of (b).

In summary, surfaces prepared using Preparation II have a much lower surface corrugation and lead to much better resolved STM data than those previously obtained using Preparation I. The main differences in these procedures are the sputtering energy and incidence angle (suggesting that minimizing surface damage while removing contaminants is of importance) and the long anneal times at high temperatures which probably serve to restore the surface composition to that of the bulk quasicrystal. We interpret the protrusions as due to material on the surface contaminants is of importance) and the long anneal times. A similar observation was recently made to explain the origin of such protrusions on d-Al-Ni-Co surfaces.

IV. REPRESENTATIONS OF SURFACES ON TERRACES IN THE GEOMETRIC MODEL M; TILING ANALYSIS OF STM IMAGES

A. A Five-Fold Terraces Mapped to the Terminations in M

In section II D we suggested new positions of five-fold terminations in the geometric model M. In this section we search for the terminations in the geometric model M on these new positions that fit to atomically resolved pictures of five-fold surfaces on particular terraces imaged by STM. In a sequence of five-fold terraces we observe a large terrace that contains a rare local configuration that we call the “Ring” (R). This configuration helps us to orient in the bulk model M, i.e., to fix the position of the R-terrace w.r.t. the five-fold z-axes. Near the R-terrace we observe the clearest terrace that we denote by “C”. A fragment of the C-terrace is shown in Fig. 8(d).

On the C-terrace local configurations of the five-fold depressions in the shape of dark Stars (dS) are observed. The strongly shining pentagonal local configurations in the form of the white Flower (wF) and the white Star pointing upwards (wSu), both parallel to the dS and in the same direction make a white picture on a dark background, see Fig. 10(a).

FIG. 10: (a) 100 Å × 100 Å high resolution STM image of the C-terrace on a five-fold surface. On the C-terrace frequently repeated local configurations such as a dark Star (dS), a white Flower (wF) and a white Star pointing upwards (wSu) parallel to the dS are marked. The Bergman polytope below the terrace (Bb), above the terrace (Ba), and the Bergman polytope dissected by the terrace (cB) are also marked. For the scale the wSu is framed by a pentagon of edge-length τD, D ≈ 4.8Å. (b) The C-terrace from (a) corresponds to the C-termination in M. Black points are atomic positions in the q-1024 plane in M (No 175 on Fig. 3) which is on the surface, grey points are in the b-1025 plane, 0.48Å below the q-1024 plane. The local atomic configurations that may present the dS, the wF and the wSu are marked. The main constituents of these configurations are the top surface of the Bergman polytopes that are in the layer below the surface (Bb), the bottom surface of the Bergman polytopes that are in the layer above the surface (Ba) and the pentagonal section of the Bergman polytopes from the layer that is dissected by the surface (cB). Scale: D = τD = 4.8Å. From the center of cB the next atomic position in the bulk is 2.04 Å below the surface.

In contrast to the C-terrace the R-terrace is not continuously (globally) clear, i.e., the STM images of the R-terrace taken on different places lead to different RDFs. Nevertheless, we observe some local configurations on the R-terrace that are clear, see Fig. 11(a). We find the white Flower (wF) and the dark Star (dS) identical to those on the C-terrace, see Fig. 11(a), but we also see a characteristic “Ring”-configuration (R) that is present on none of the other observed terraces. The terrace is therefore denoted the R-terrace. In the R-terrace there is also a configuration which we call the white Star pointing downwards (wSd), it is rotated 180° w.r.t. the wSu that we observe on the C-terrace.

As we stated the areas of both R- and C-terrace are large and they appear in a local upward sequence of steps ml(R)ml(C), where m ≈ 4.08Å and l ≈ τm. On the q-planes of the geometric model M we find a rare atomic configuration that may represent a local Ring-configuration on the STM-image of the R-terrace, compare Figs 11(a) and (b). We determine the coding of the ring-configuration (R) in E⊥ and demand that the q-plane containing the Ring-configuration is to be found in an upward sequence of the q-planes ml(R)ml(C) on the new positions (shifted by 4.08Å, see section II D), and both R- and C-plane are to be among the planes from the decorated Fibonacci sequence. From these conditions we find the coding area in E⊥ along z⊥ of the R-plane to be in the interval z⊥ ∈ (0.198, 0.337)τ[7] marked on Fig. 11. In a patch of the geometric model M that spreads along z∥-axes in an interval of 1195 Å
we find only 15 representatives of the R-plane that fulfill all conditions mentioned above. We choose the q-1037 plane (No 178 on Fig. 13), the plane that is coded in \( E_\perp \) by \( z_\perp = 0.192\tau^2\overline{5} \), see Fig. 6. The corresponding C-plane is then q-1024 (No 175 on Fig. 13) coded by \( z_\perp = 0.323\tau^2\overline{5} \), see Fig. 6. In Fig. 12 the coding windows of the R- and the C-plane are shown. This pair of R- and C-planes (one of 15 pairs in the model-patch) are taken not far from the estimated model-plane S8 for Schaub’s terrace No. 8 on a new position q-1128 (No 193 on Fig. 13) coded by \( z_\perp = 0.211\tau^2\overline{5} \), see Fig. 6.

![FIG. 11: (a) 75 Å × 75 Å STM image of the R-terrace. The local configurations Ring (R), dark Star (dS) and white Star pointing downwards (wSd) are framed by three pentagons of edge-lengths \( \tau^2D \), \( \tau^2D \) and \( \tau D \) respectively, where \( D \approx 4.8 \AA \). On a bigger STM image of the R-termination a full white Flower (wF) can be seen also. (b) The R-terrace from (a) corresponds to the R-termination in \( M \). Black points are atomic positions in q-1037 plane in \( M \) (No 178 on Fig. 4) which is on the surface, grey points are in b-1038 plane, 0.48Å below the q-1037 plane. The local configurations of atomic positions that may represent the dark Star (dS), the white Flower (wF) and the white star (wSd) anti-parallel to the dark Star (dS) are marked. Scale: \( D = \tau d = 4.8 \AA \). In the centre of the dark Star the nearest atomic position is 2.04 Å below the surface. In the q-1037 plane there are empty “streets”, \( \Delta = 4.56 \AA \) broad.](https://example.com/figure11)

![FIG. 12: In \( E_\perp \) the windows of the top (q-)planes in R- and C-terminations, \( W_R \) and \( W_C \), respectively. Over them is plotted (i) the window of the tiling \( P_1 \) of edge-length 4.8\( \AA \) (in \( E_\parallel \)) denoted by \( W_{T(p_1)} \). It is the maximal window of \( P_1 \), such that \( W_{T(p_1)} \subset W_C \) and (ii) the window of the terrace \( T(p_1) \), of edge-length 7.8\( \AA \) (in \( E_\parallel \)), denoted by \( W_{T(p_1)} \). It is the maximal window of \( P_1 \), such that \( W_{T(p_1)} \subset W_C \subset W_C \). The scale for the figure is set by the decagon \( W_{T(A_4)} \), which is the window of the tiling \( T(A_4) \) with edges \( d = \tau^{-1}D \) and \( D = 4.8 \AA \) (in \( E_\parallel \)). (a) For the biggest possible window of \( P_1 \) in \( W_{T(p_1)} \) see Fig. 6(a) in section II B.)](https://example.com/figure12)

![FIG. 13: A decorated Fibonacci sequence \( (s = 2.52 \AA, m = 4.08 \AA, l = 6.60 \AA) \) of the q-planes along the \( z_\parallel \) (five-fold axes) of type \( \pm 1, \pm 2, \pm 3, \pm 4, \pm 5 \) in \( M \) on the old positions, see Ref. 1. Relative to these positions the stacked layers of the Bergman polytopes are drawn with their relative densities. The representative planes of the large R-, C- and S8-terrace are marked on the new positions. The –4.08Å shift from the old to the new positions is indicated by arrows.)](https://example.com/figure13)

As we have stated, in contrast to the R-terrace, the C-terrace is uniformly clear and it has a unique radial distribution function (RDF). Fig. 14 (top) corresponds to the RDF calculated from the high resolution STM image of Fig. 1(d) (identical to the RDF shown in Fig. 3(d)). Maxima are found at 7.3, 12.1, 19.4, 24.2, 31.1, and 38.0 Å (± 0.3 Å). The radial distribution function calculated from the C-plane q-1024 (No 175) of the geometric model \( M \) (shown in Fig. 14 bottom), is very similar, the main differences being the presence of a double peak at 15 Å, and some extra structure at higher distances. The correspondence with the largest intensity peaks is however very good.

To the C- and the R-planes of type q, there correspond C- and R-terminations, which are pairs of q- and b-planes at the surface separated by a vertical distance of 0.48Å. All local patterns observed on the C-terrace and the R-terrace can be mapped to the model-terminations, the C(lear)-termination and the R(ing)-termination, respectively, see Figs 14(b) and 14(b). These patterns are mapped to the local atomic configurations on model-terminations that contain groups of atoms in the shape of pentagons related to Bergman polytopes that (i) either dissect the termination (cB) (some of them are in the central parts of dS); or (ii) are below the termination (Bb) (some of them are in dS, wF, R, wSd); or (iii) to the Bergman polytopes that are above the termination (Ba) (in wSu). For this see Figs 14(b), 14(b) and 14.

### B. The Tiling P1 on Five-Fold Surfaces

In order to extract information from the STM images, we have employed a tiling approach in Ref. 22. In Ref. 22 this consisted of connecting points of high contrast on the STM image to create pentagons. The filling-in of the image using pentagons led to a Penrose (P1)-like tiling of the experimental plane (with an edge-length of 7.8Å).

Here we will reconstruct exact patches of the P1 tiling on the STM images of both R- and C-terrace images (see Figs 13 and 10) and on corresponding model-planes (not shown).

The coding regions of P1 tilings with minimal edge-lengths on q-planes are marked on Fig. 4. The tiling P1 with edge-length 7.8Å is coded in the interval \( z_\parallel \in (\tau^{-1}, \tau^{-1})[\tau^2\overline{5}] \) and that with edge-length 4.8Å in the interval \( z_\parallel \in (\tau^{-3}, \tau^{-3})[\tau^2\overline{5}] \).

From the coding of the q-planes of the C-, S8- and R-terminations \( z_\parallel^C = 0.192\tau^2\overline{5} \), \( z_\parallel^{S8} = 0.211\tau^2\overline{5} \) and \( z_\parallel^R = 0.323\tau^2\overline{5} \) we conclude that the q-1024 plane (No. 175 in Fig. 4) of the C-termination and the q-1128 plane (No. 193 in Fig. 4) of the S8-termination in \( M \) allow a P1 tiling of minimal edge-length 4.8Å, and the q-1037
plane (No. 178 in Fig. 13) of the R-termination allows a P1 tiling of minimal edge-length 7.8 Å. (See also in Fig. 13 the coding windows of P1 tilings with edge-lengths 4.8 Å and 7.8 Å plotted over the coding windows of the q-1024 plane of the C-termination and the q-1037 plane of the R-termination).

An exact patch of the tiling P1 can be exactly placed on the q-plane of a model termination as follows: (i) Plot the window of the P1 tiling, \( W_{P1} \), of the maximal possible size such that \( W_{P1} \subseteq W_{q-pl} \), where \( W_{q-pl} \) is the coding window of the surface q-plane in the model \( \mathcal{M} \). For the biggest possible window of P1 in \( W_{\tau^*(A_1)} \) see Fig. 13(a) in section II B. (ii) Mark all atomic positions coded by the points in the window \( W_{P1} \) in \( \mathbb{E}_\parallel \). This set of points uniquely determines the P1 tiling on the model q-plane. The procedure is evident. In contrast, for an STM image of a terrace we have to proceed locally. If the plane is very clear and the window \( W_{P1} \) can be tightly placed in the corresponding window \( W_{q-pl} \) we can reconstruct an exact patch of the P1 tiling by trial and error. A probable exact patch of the tiling P1 with minimal edge-length of 7.8 Å is reconstructed on an STM image of the R-terrace, in Fig. 15.

FIG. 15: 75 Å × 75 Å segment of an STM image of the R-terrace with a superimposed exact patch of the P1 tiling of edge-length 7.8 Å.

The q-1024 plane related to the surface of the C-termination is very dense, and although we could theoretically place the P1 tiling of minimal edge-length 4.8 Å (see Fig. 12), we have managed to reconstruct only an exact patch of P1 tiling of edge-length 7.8 Å on the STM image of the C-terrace, see Fig. 16. For this purpose we apply an image enhancement technique to the data of Fig. 16(d) in order to even out experimental contrast variations (inherent in the use of the STM technique which measures electron charge density at the surface rather than nuclear coordinates) and to reduce experimental noise. The procedure is based on Fourier filtering and consists of taking a fast Fourier transform of the image, and then enhancing obvious Bragg reflections with unique \( k \)-values and removing experimentally-induced diffuse features due to noise. This modified frequency space representation is then Fourier transformed to obtain the filtered image shown in Fig. 16(a). The result of this procedure is to strongly enhance features in the image corresponding to the selected \( k \)-values. The procedure is essentially identical to that used by Beeli and co-workers in the enhancement of High Resolution Transmission Electron Microscopy (HRTEM) images [8].

In the enhanced image the white spots that we interpret as the images of atomic positions are almost as sharp as in the model plane q-1024 from the C-termination, see Fig. 10(b). We find a patch of exact P1 tiling of edge-length 7.8 ± 0.2 Å that can be easily superimposed on the enhanced image, see Fig. 16(a). Fig. 16(b) shows this tiling superimposed on the unenhanced STM image.

C. Densities of Five-Fold Planes and Terminations

In Table II we compare the densities of the R-, C- and S8-terminations, and also the densities of single (q- and b-) planes contained in each termination on the old and the new positions. It is evident that the densities of

| termination | R | S8 | C | average |
|-------------|---|----|---|---------|
| \( \rho_{(q)} \) [Å\(^{-2}\)] | 0.087 | 0.084 | 0.082 |
| \( \rho_{(b)} \) [Å\(^{-2}\)] | 0.026 | 0.008 | 0.007 |
| \( \rho_{(q+b)} \) [Å\(^{-2}\)] | 0.113 | 0.092 | 0.089 | 0.098 |
| \( \rho_{(q)} \) [Å\(^{-2}\)] | 0.059 | 0.074 | 0.076 |
| \( \rho_{(b)} \) [Å\(^{-2}\)] | 0.076 | 0.063 | 0.060 |
| \( \rho_{(q+b)} \) [Å\(^{-2}\)] | 0.135 | 0.136 | 0.136 | 0.136 |

V. CONCLUSIONS

We have presented two atomically resolved, high resolution STM images of large and flat terraces on the five-
fold $\text{Al}_{70}\text{Pd}_{3}\text{Mn}_{2}$ surface. We have mapped these surfaces to the five-fold terminations in the geometric model $\mathcal{M}$ such that they form a decorated Fibonacci sequence, and their average atomic density is in agreement with the LEED measurements of Gierer et al.\textsuperscript{11} Due to the polytopal windows of the geometric model $\mathcal{M}$ all terminations turn out to have equal and simultaneously maximal densities. These new terminations in $\mathcal{M}$ are placed 4.08 Å lower than in the work of Ref.\textsuperscript{13}. On the present STM images the dark pentagons appear as the dark Stars. At the new positions of the model-termination planes the patterns of dark pentagonal holes are the same as in Ref.\textsuperscript{13} but now each dark hole is of an appropriate size. At the new positions the surface terminations dissect the most dense Bergman layers in the model $\mathcal{M}$. The local patterns on STM images are present in the model terminations and are related to the Bergman layers above (if one exists), below and dissected by the termination. Dissected Bergman polytopes correspond to the dark Stars. The edge-lengths of superimposed exact patches of the Penrose P1 tiling on two STM images (corresponding to pentagons of height equal to $12 \pm 0.36$ Å) are shown to be in agreement with the bulk model $\mathcal{M}$ based on the tiling $\tau T^{+2P[4]}$.\textsuperscript{14}

VI. ADDENDUM

Since this manuscript was submitted for publication another paper containing STM results has been published, see Ref.\textsuperscript{12}. We note that those authors also conclude that the $\text{i-Al-Pd-Mn}$ surface is a termination of the bulk structure.

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44 The Bergman polytope is a dodecahedron with particular concave pentagonal faces, see Ref. 16.
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46 A point $q \in D_6^{\text{rec}}$ is composed of 6 integers $(n_1, \ldots, n_6)$, such that $\sum_{i=1}^6 n_i = \text{even}$. These prototiles can be uniquely reconstructed from the point set of atomic positions.
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