We consider clean surfaces of quasicrystals by comparing their STM (scanning tunneling microscopy) and SEI (secondary electron imaging) images to the bulk terminations in the deterministic atomic models. A bulk model is defined as an ideal quasiperiodic tiling with atomic decoration on a finite number of tiles. In Section II an STM image of a decagonal quasicrystal is compared to the Burkov model \( \mathcal{M}(T^{+}(A_4)) \), based on a decagonal tiling \( T^{+}(A_4) \), see Ref.\(^{\text{a}}\). In section III STM and SEI images of an icosahedral quasicrystal are compared to the model \( \mathcal{M}(T^{2}(2F')) \), based on icosahedral tiling \( T^{2}(2F') \), see Ref.\(^{\text{b}}\). The clean surfaces, that we study, are considered not to be reconstructed.

In our previous work on terrace-like clean surfaces of icosahedral quasicrystals we tried to define the 5fold terminations based on a decagonal tiling \( \mathcal{M}(T^{+}(A_4)) \), see Refs.\(^{\text{c}, \text{d}}\). In Ref.\(^{\text{e}}\) we adopt the Bravais’ rule of maximum density, allowing that instead of a single atomic plane a layer of atomic planes may form a bulk termination.

I. SURFACES OF DECAGONAL QUASICRYSTALS

Decagonal Al\(_{65}\)Cu\(_{15}\)Co\(_{20}\) (d-AlCuCo) is periodic in \( z \)-direction\(^{10}\) with periodicity \( t=4.13 \) Å. The \( z \)-direction is orthogonal to the quasiperiodic decagonal \( x-y \) plane. The phase crystallizes in a shape of long thin decagonal prisms, with the 2fold surfaces considerably larger than the 10-fold surfaces, see Fig.\(^{\text{I(a)}}\). The size of the surface area is evidently a parameter of its stability. In Fig.\(^{\text{I(b)}}\), over the image of the 10fold surface\(^{\text{10}}\), we determine the positions of possible 2fold surfaces, orthogonal to the 10fold surface. In the model \( \mathcal{M}(T^{+}(A_4)) \) \( \text{t=4.18 } \text{Å} \) we investigate the densities of the “thin”, 2fold layers containing 2 atomic planes. Among these, the most dense one is a 0.47 Å-layer of the density \( \rho_{2} = 0.124 \text{ Å}^{-2} \). Comparing it to the much smaller 10fold surface, which is of the density \( \rho_{10} = 0.146 \text{ Å}^{-2} \), we conclude that the 0.47 Å-layer can not represent the 2fold termination. But, on some positions in the bulk these layers appear in pairs, 0.29 Å apart. Such, a rather “thick” 1.23 Å-layer of 4 planes on mutual small distances (see Fig.\(^{\text{I(c)}}\)) is a candidate for a terminating layer. These layers appear on distances mutually scaled by the factor \( \tau = (1 + \sqrt{5})/2 \) \( (12.3 \text{ Å}, 19.9 \text{ Å}, 32.2 \text{ Å}, 52.1 \text{ Å} \ldots \) as in Fig.\(^{\text{I(c)}}\), in excellent agreement with those found on the STM image (21 Å, 31 Å, 54 Å, see Fig.\(^{\text{I(b)}}\)).

II. SURFACES OF ICOSAHEDRAL QUASICRYSTALS

A feature of the surface of i-AlPdMn, not accounted for by the “thin” layer analysis\(^{3,4}\), is that not all types of maximally dense layers appear as surfaces: for example, (\( q, b \)) layers\(^{4} \) 0.48 Å apart, are seen in 5fold surfaces but equally dense (\( b, q \)) layers, also 0.48 Å apart, are not. If both kind of layers were possible terminations, the sequence of much shorter terrace heights, than observed, could appear. If one chooses to define a termination incorporating the neighboring planes too, as we did in decagonal case (in Section I), one could introduce a “thick” layer as a bundle of high density planes (or thin, plane-like layers). A 5fold termination can be considered to be a “thick” layer consisting of a (\( q, b \)) layer and a (\( b, q \)) layer, each with the spacing 0.48 Å. Such a layer contains 4 planes with spacings: \( q \)-plane, 0.48 Å, \( b \)-plane, 1.56 Å, \( b \)-plane, 0.48 Å, \( q \)-plane. For a bundle we define an effective (averaged) density of within contained “thin” layers/planes \( \rho_{q,b}(z_{\perp}) = (\rho_{q1}(z_{\perp}) + \rho_{q2}(z_{\perp}))/2 + (\rho_{b2}(z_{\perp}) + \rho_{b3}(z_{\perp}))/2 \).

As we see in Fig.\(^{\text{II(a)}}\), whereas for the thin-layer concept the width of the support of the plateau is approximately \( \frac{2\tau^2}{1+\tau^2} \) broad, and consequently encodes the Fibonacci sequence of terrace heights \( S = 4.08 \text{ Å} \) and \( L = \tau S = 6.60 \text{ Å} \) \( \tau = (1 + \sqrt{5})/2 \), in the thick-layer concept the width is exactly \( \frac{2\tau}{1+\tau^2} \) \( \tau \geq \) larger terrace heights, i.e. \( L = 6.60 \text{ Å} \) and \( L + S = \tau L = 10.68 \text{ Å} \). Whereas on the clean surfaces, obtained at lower annealing temperature, even the terrace height \( \tau^{-1} S = 2.52 \text{ Å} \) appears\(^{16}\) on the surfaces ob-
The height of the plateau of the graph \( \rho_{5f}(z) \) (see Fig. 2(a)) defines the densities of the “thick” layer terminations to be 0.134 Å\(^{-2} \). The 5fold layers intertwining the terminations are of densities not higher than 0.072 Å\(^{-2} \). It is also a fact, that the density graphs of the “thin” and the “thick” layers have a strong overlap, see Fig. 2(a). Hence, almost any \((q, b)\) “thin” layer termination occurs within such a \((q, b, b, q)\) “thick” layer termination. The same holds true for any icosahedral quasicrystal described by the \( M(T^{\star}(2F)) \) model.

Above each termination, there is a 2.04 Å gap, if we dare to neglect an \( a \)-plane of a density smaller than 0.013 Å\(^{-2} \). But, if each gap of 2.04 Å in the model \( M(T^{\star}(2F)) \) would be declared as a criterion of a termination to appear below it, as in Ref. 15, the 2.04 Å terrace heights, that were not observed, should appear as well. However in the model \( M(T^{\star}(2F)) \) there is a low density 5fold layer \((b, a, q, b, q, a, b)\) (see Fig. 2(b)), 4.08 Å broad. The width of the cavity on the density graph of these layers, \( W = \frac{2}{\tau^2} \), encodes a Fibonacci sequence with the intervals \( \tau L = 10.68 \) Å and \( \tau^2 L = 17.28 \) Å. These are the minimum density layers of equal, 0.041 Å\(^{-2} \) density, placed in the model over a subsequence of the terminations. Hence, the minimum density layer sequence alone can not define the terminations, because
the standard distance along a 2fold axis line), which is a single, (full line). The plateau (maximum density) of the graph defines the planes with spacings:

plane, 2fold terminating atomic fines the effective densities of terminations to be more than 0.079 Å⁻² (< 0.086 Å⁻²). The small 2fold terraces, or rather the pits within the big terraces (see Fig. 3(a) and 3(c) in Ref. 2) may be explained by the comparatively large distances between the atomic planes inside of the “thick” terminating layer (1.5 Å, 2.4 Å and 3.9 Å). These excellently reproduce the measured values (2.4 Å and 3.6 Å), see Fig.3(a) and 3(c) in Ref. 2.

In the model $M(T^{(2F)})$ there is a low density 2fold layer $(bq, bq)$: 0.92 Å gap, $bq$-plane, 0.57 Å, $bq$-plane, 0.92 Å gap (see Fig. 2(b)). The width of the cavity on the graph of these layers, $W = (\tau/2)\mathfrak{S}$, encodes a Fibonacci sequence with the intervals $\tau^{-1} S = 3.9$ Å and $S = 6.3$ Å. These are the minimum density layers of almost equal density, somewhat above 0.063 Å⁻². A member of a subsequence of these layers is placed over each 2fold termination. Nevertheless, in the 2fold case the minimum density layer sequence alone cannot define the terminations, because it predicts by $\tau^{-1}$ shorter terrace heights between the large 2fold terminations, than observed.

The 3fold terminations could also be modeled as “thick” layers of atomic planes in $M(T^{(2F)})$, see table I. But, inspecting the intertwining 3fold layers, we see that these are of the densities comparable to the “terminating” ones. We also know that the 3fold surfaces facet readily, and some correlated STM measurements, (as those in Fig.3(a) and 3(c) of Ref. 2) for the 3fold surfaces do not exist so far.

On the STM measurements it is in general hard to judge whether “thin” layer or “thick” layer terminations best model the physical surfaces. However, in the 5fold case, the “thick” layer concept removes the contradiction with respect to the Bravais’ rule, that some, equally dense layers do not appear on the surfaces, see Ref. 2. In the 2fold case the “thick” layer concept is evidently better, it treats differently the large terraces compared to the small pits inside. That the effective densities of the 2fold terminations are somewhat lower than the densities of some single 2fold planes is not contradictory, because these are included in the most dense layers.

Fig. 3(a) shows the secondary-electron patterns obtained from the clean pentagonal surface of a quasicrystalline Al₇₀Pd₂₀Mn₁₀ sample. Secondary-electron images (SEI) represent an orthogonal projection to the sphere of the sym-

![FIG. 3: (a) (top) Density graph $\rho_{2f}(z_\perp)$ of the “thick” 2fold layers (full line). The plateau (maximum density) of the graph defines the terminations. It is compared to the “thin” layer termination (dotted line), which is a single, $abq$-plane termination. The symbol $\mathfrak{S}$ is the standard distance along a 2fold axis $z_\perp$ in the coding space $E_\perp$. (b) (bottom) Density graph of the 2fold layer $(bq, bq)$. The cavity defines a sequence of the minimum density layers in $M(T^{(2F)})$, of which a subsequence is situated above all the 2fold terminations.](image)

It does not reproduce the pairs of large terraces 6.60 Å apart, which were frequently observed.

In the case of 2fold surfaces, we may replace a single dense 2fold terminating atomic $abq$-plane by a layer of 4 atomic planes with spacings: $abq$-plane, 1.48 Å, $bq$-plane, 0.92 Å, $bq$-plane, 1.48 Å, $abq$-plane. For a bundle we define an effective (averaged) density of planes

$$\rho_{2f}(z_\perp) = (1/4)\{\rho_{abq_1}(z_\perp) + \rho_{bq_1}(z_\perp) + \rho_{bq_2}(z_\perp) + \rho_{abq_2}(z_\perp)\},$$

For this “thick” 2fold layer the peak of $\rho_{2f}(z_\perp)$ is a perfectly flat plateau, see Fig. 3(a). The height of the plateau defines the effective densities of terminations to be 0.086 Å⁻², see Table I. The support of the width of the plateau equals $W = (1/2)\mathfrak{S}$ and encodes the Fibonacci sequence of 2fold terminations with the terrace heights $S = 6.3$ Å and $L = \tau S = 10.2$ Å. The standard distances along 5, 2 and 3fold axes in icosahedral structures are $\mathfrak{S} / \sqrt{\tau + 2} = \mathfrak{S} / 2(= 1/\sqrt{2(\tau + 2)}) = \mathfrak{S} / \sqrt{5}$, where $\tau = (1 + \sqrt{5})/2$. The heights of the larger 2fold terraces were measured to be $S = 6.2$ Å and $L = 9.5$ Å (see Fig. 3(a) and 3(c) in Ref. 2), in good agreement with the predicted values. The 2fold layers intertwining the terminations are of densities not higher than 0.079 Å⁻² (< 0.086 Å⁻²). The small 2fold terraces, or rather the pits within the big terraces (see Fig. 3(a) and 3(c) in Ref. 2) may be explained by the comparatively large distances between the atomic planes inside of the “thick” terminating layer (1.5 Å, 2.4 Å and 3.9 Å). These excellently reproduce the measured values (2.4 Å and 3.6 Å), see Fig.3(a) and 3(c) in Ref. 2.

| TABLE I: Relative and absolute densities of the planes and layer terminations orthogonal to 5, 2 and 3fold symmetry axes in $M(T^{(2F)})$ of i-AlPdMn. The corresponding data for i-AlCuFe are similar. |
|-------------------------------|-------------|-------------|-------------|
| Densest planes (abs.)         | 0.086 Å⁻²  | 0.101 Å⁻²  | 0.066 Å⁻²  |
| Densest “thin” layers (abs.)  | 0.133 Å⁻²  | 0.101 Å⁻²  | 0.066 Å⁻²  |
| Densest “thin” layers (rel.)  | 1          | 0.76       | 0.50       |
| Densest “thick” layers (abs.) | 0.134 Å⁻²  | 0.086 Å⁻²  | 0.058 Å⁻²  |
| Densest “thick” layers (rel.) | 1          | 0.64       | 0.44       |
Fig. 4: (a) (left) Secondary-electron pattern obtained from the pentagonal surface of a single icosahedral Al$_{20}$Pd$_{20}$Mn$_{10}$ quasicrystal. The center of the pattern is obscured by the shadow of the electron gun used for the excitation. The edge of the screen corresponds to $\theta = 52^\circ$. (b) (right) Calculated secondary-electron pattern based on the single scattering approximation of electrons using model $\mathcal{M}(\mathcal{T}^{\ast}(2F))$.

A quantum mechanical single-site scattering calculation$^{12}$ is a faithful representation of the SEI pattern because it accounts for the wave nature of the secondary electrons. Fig. (b) illustrates the results of the calculation$^{12}$ using the coordinate set of the model $\mathcal{M}(\mathcal{T}^{\ast}(2F))$. This approximation overestimates the scattering intensity along chains of atoms$^{12}$ but suffices for purposes, since our interest is mainly in the presence or absence of bands on the screen. As in case of crystals$^{12}$ the band width is inversely proportional to the spacing of crystallographic planes, and the band width is related to the distance of interatomic planes$^{12}$. The observed band widths reveal that the inter-planar distances of the highly dense 2fold planes are broader than those of the 5fold planes/plane-like layers by a factor 1.6. In 5fold case, from the model we predict the distance $d_5 = \tau/(\tau + 2) = 2.04$ Å, which is the distance between the highly dense $(q,b)$ and the $(b,q)$ plane-like layers in the terminating thick layer $(q,b,b,q)$: $2.04$ Å $= 0.48$ Å + 1.56 Å, see also Ref. $^{18}$. In the 2fold case, between the highly dense planes in the above defined “thick” layer, appears once the distance of 0.92 Å and twice the distance of 1.48 Å. Hence, an average distance between the highly dense planes is $d_2 = \frac{\tau}{3\sqrt{\tau + 2}} = 1.29$ Å. And their ratio is $d_5/d_2 = 3/\sqrt{\tau + 2} \approx 1.6$.

The SEI method does not determine the bulk termination, (it is testing the bulk circa 30 Å below the surface). However, in the case of the ordinary crystals, the Kikuchi bands are related to the most dense atomic planes, and we show that the same holds true in the case of quasicrystals as well. Hence we may claim that SEI images are supporting the thick atomic layers of the high effective density to be the bulk terminations, if the Bravais’ rule should be valid in quasicrystals as well. The not existing 3fold Kikuchi bands are also supporting the model $\mathcal{M}(\mathcal{T}^{\ast}(2F))$, in which we find that the atoms collected by the 3fold planes are almost uniformly distributed among these, without the notable repetitive layers of higher densities.

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