Thick atomic layers of maximum density as bulk terminations of quasicrystals

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Clean surfaces of quasicrystals orthogonal to the directions of the main symmetry axes have a terracelike appearance. We extend Bravais' rule for crystals to some common quasicrystals by allowing thick layers of atomic planes, instead of single atomic planes/thin layers, to be candidates for terminations in bulk model.

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We study clean surfaces of quasicrystals by comparing their scanning tunneling microscopy (STM) and secondary electron imaging (SEI) images with bulk terminations in deterministic atomic models.[1–3] We investigate decagonal Al-Cu-Co (*d*-AlCuCo) in Sec. I and icosahedral Al-Pd-Mn (*i*-AlPdMn) in Sec. II.

In Ref. 3 we adapted Bravais' rule of maximum density by allowing thin, planelike atomic layers in quasicrystals to be treated as single planes for density comparisons. In that framework we gave a possible explanation of the experimental fact that, although the twofold planes in the model[2,3] are more dense than the fivefold planes, the fivefold surfaces are the most stable in icosahedral quasicrystals.[4] In the same paper[3] we also announced the "thick layer" concept that we elaborate here. With the "thick layer" concept we consider a bundle of dense atomic planes in the bulk, not necessarily extremely close together, as a candidate for a termination. We show that only "thick" layers can terminate the bulk of *d*-AlCuCo in the twofold directions. Also, SEI images indicate that certain "thick" fivefold and twofold layers are favored as terminations of *i*-AlPdMn. In particular, the twofold terracelike surfaces of *i*-AlPdMn containing pits are perfectly explained in this framework. Some recent investigations on wetting of decagonal quasicrystals favor the "thick" layer concept as well.[5]

Following a suggestion of Sharma *et al.*,[6] that a gap in the bulk might define a termination, we introduce a *minimum* density rule on low density "thick" atomic layers as well and show that, in the framework of the model of *i*-AlPdMn,[2,3] such a rule does not match the observed step heights on either the twofold or fivefold surfaces.

I. SURFACES OF DECAGONAL QUASICRYSTALS

Decagonal $Al_{65}Cu_{15}Co_{20}$ (*d*-AlCuCo) is periodic in the z direction,[7] 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 twofold surfaces considerably larger than the tenfold surfaces, see Fig. 1(a).

The size of the surface area is evidently a parameter of its stability. In Fig. 1(b), over the image of the tenfold surface,[7] we determine the positions of possible twofold surfaces, orthogonal to the tenfold surface. In the model $\mathcal{M}(\mathcal{T}^{*(A_4)})$[1] (with periodicity $t=4.18$ Å), based on a decagonal tiling $\mathcal{T}^{*(A_4)}$,[9] we investigate the densities of the "thin", twofold layers containing two atomic planes. Among these, the most dense one is a 0.47-Å layer of the density $\rho_2^{0.47\ \text{Å}}=0.124\ \text{Å}^{-2}$. Comparing it to the much smaller tenfold surface (actually fivefold), which is of the density $\rho_{10}=0.146\ \text{Å}^{-2}$, we conclude that the 0.47-Å layer can not represent the twofold 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 four planes on mutual small distances [see Fig. 1(c)] is a candidate for a terminating layer. These layers appear on distances mutually scaled by the factor $\tau=(1+\sqrt{5})/2$ [12.3,19.9,32.2,52.1,… Å, as in Fig. 1(c)], in excellent agreement with those found on the STM image [21, 31, 54 Å, see Fig. 1(b)].

II. SURFACES OF ICOSAHEDRAL QUASICRYSTALS

A. Model of icosahedral quasicrystals

The deterministic model of *i*-AlPdMn (and also of *i*-AlCuFe), denoted by $\mathcal{M}(\mathcal{T}^{*(2F)})$,[2,3] is based on the tiling $\mathcal{T}^{*(2F)}$.[10] The model is a superposition of three icosahedral quasilattices q, a, and b, of atomic positions in the physical space $\mathbb{E}_\parallel$. For definition of q, a, and b atomic positions, see Table I in Ref. 3. Each quasilattice is defined by a corresponding "atomic surface" (the "window") in the coding space, $\mathbb{E}_\perp$ shown in Fig. 2.

To specify the scale in the model $\mathcal{M}(\mathcal{T}^{*(2F)})$ we use standard distances, denoted by ⑤, ②, and ③ along the fivefold, twofold, and threefold axes, respectively, which are related by $③/\sqrt{3}=⑤/\sqrt{\tau+2}=②/2[=1/\sqrt{2(\tau+2)}]$, where $\tau=(1+\sqrt{5})/2$. The standard distances are used both, in the observable space $\mathbb{E}_\parallel$ and in the coding space $\mathbb{E}_\perp$. The standard distance ⑤$(=1/\sqrt{2})$ in $\mathbb{E}_\parallel$ is set to be 4.561 Å for *i*-AlPdMn and 4.465 Å for *i*-AlCuFe.

B. Thick atomic layers as terminations

A feature of the fivefold terminations of *i*-AlPdMn, not accounted for by the "thin" layer analysis,[3] is that not all types of maximally dense layers appear as surfaces: for example, (q,b) layers, 0.48 Å apart, are seen in fivefold sur-

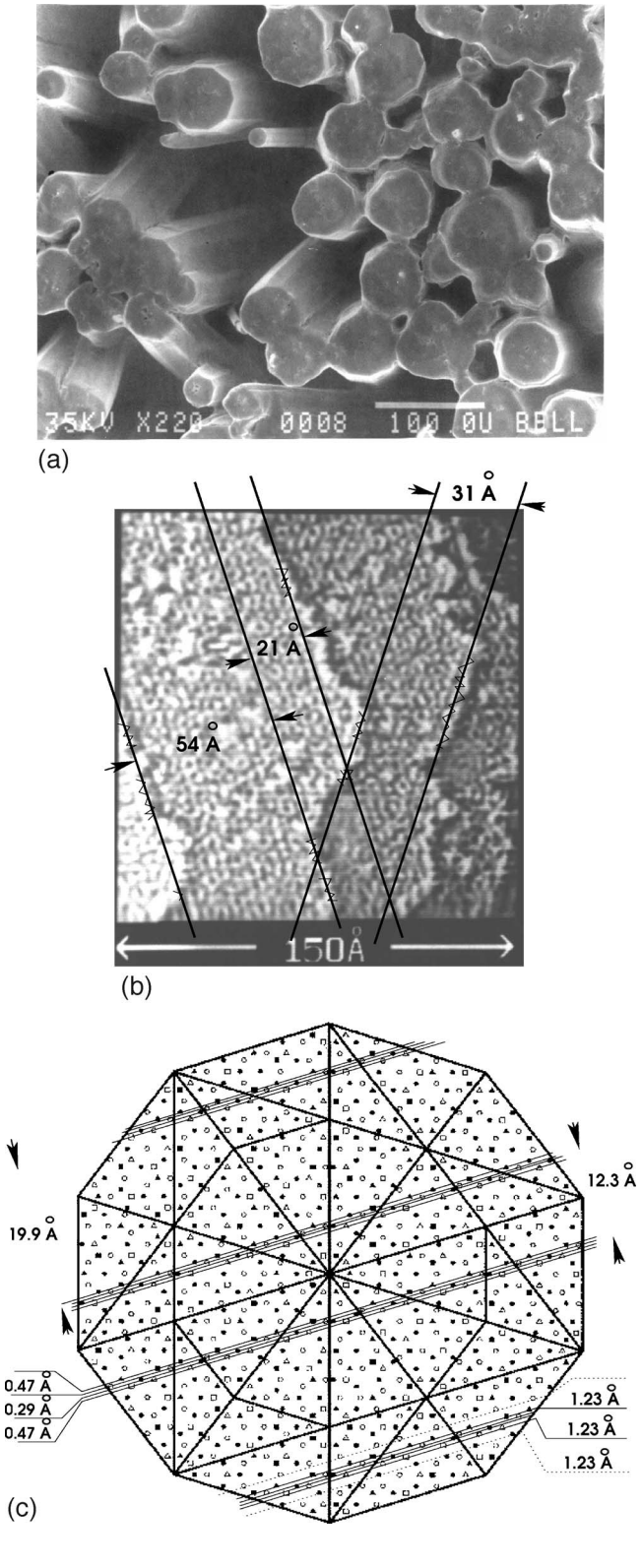

FIG. 1. (a) Long, thin decagonal prisms (Ref. 8) of the *d*-AlCuCo; (b) estimated positions of twofold surfaces on an STM image of the tenfold terracelike surface of *d*-AlCuCo; (c) twofold bulk terminations in the model $\mathcal{M}(\mathcal{T}^{*(A_4)})$ marked on a tenfold one (Ref. 9).

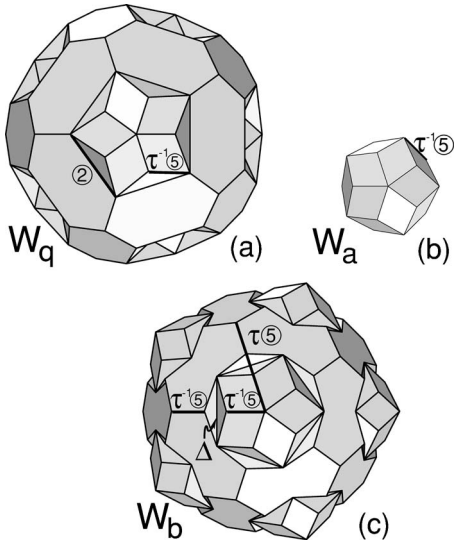

FIG. 2. The windows W_q, W_a, W_b are polyhedra in the coding space $\mathbb{E}_\perp$. They define the geometric model $\mathcal{M}(\mathcal{T}^{*(2F)})$ of atomic positions based on the icosahedral D_6 module M_F. The model $\mathcal{M}(\mathcal{T}^{*(2F)})$ describes both *i*-AlPdMn and -AlCuFe. (a) W_q with edge lengths $\tau^{-1}⑤$ and $②=2⑤/\sqrt{\tau+2}$. (b) W_a is a triacontahedron of edge length $\tau^{-1}⑤$. (c) W_b is obtained by taking the marked tetrahedra (Δ) away from the triacontahedron of edge length $\tau⑤$. The tetrahedron Δ has two mirror symmetry planes and edges of lengths $\tau^{-1}⑤$, $\tau^{-2}⑤$, and ②. The windows fulfill the closeness condition. The volumes of the windows are in the proportion $\mathrm{vol}(W_b):\mathrm{vol}(W_q):\mathrm{vol}(W_a)=(6\tau+8):(8\tau+2):1$.

faces 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 Sec. I), one could introduce a "thick" layer as a bundle of high density planes (or thin, planelike layers). A fivefold 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 four 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

$$\rho_{5f}(z_\perp)=[\rho_{q_1}(z_\perp)+\rho_{b_1}(z_\perp)]/2+[\rho_{q_2}(z_\perp)+\rho_{b_2}(z_\perp)]/2.$$

Whereas the density of the bundle in dependence of it's position in the bulk along the symmetry axis ($z_\parallel$) in $\mathbb{E}_\parallel$ is not a function, in the coding space $\mathbb{E}_\perp$ it is a function[3] of $z_\perp$, the density graph $\rho(z_\perp)$. The area below the plateau along $z_\perp$ (the support of the plateau) marks the layers with the equal maximum densities, the terminations. Each module point in the support along fivefold symmetry axes $z_\perp$ in $\mathbb{E}_\perp$ is 1-1 to $z_\parallel$, a position of the penetration of fivefold symmetry axis (in $\mathbb{E}_\parallel$) into a single terminating layer.

One could also bundle the dense (b,q) and (q,b) planelike layers into a "thick" layer (b,q,q,b), see Fig. 3(b). Such a layer contains actually five planes with spacings: b plane,

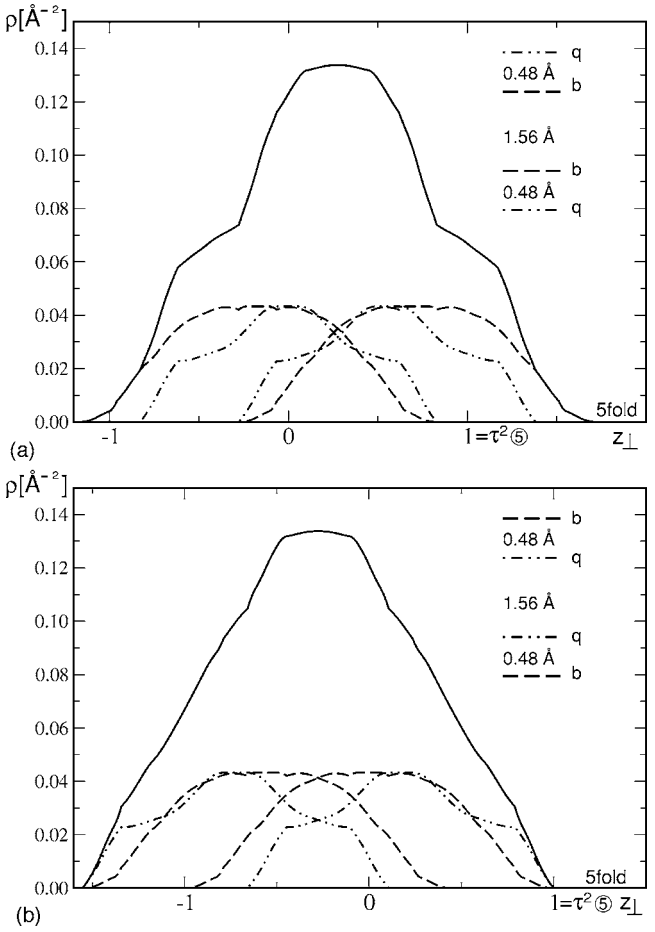

FIG. 3. (a) Density graph $\rho_{5f}(z_\perp)$ of the "thick" fivefold (q,b,b,q) layers, with spacings as in the image. The width of the support of the plateau of the graph [see Fig. 4(a)] may define the Fibonacci sequence of the terminations with step heights $S=[2\tau^2/(\tau+2)]⑤=6.60$ Å and $L=\tau S=10.68$ Å, $\tau=(1+\sqrt{5})/2$. The symbol ⑤ is the standard distance along a fivefold axis. (b) Density graph $\rho_{5f}(z_\perp)$ of the "thick" fivefold (b,q,q,b) layers, with spacings as in the image. The supports of the plateaus in case (a) and (b) are equaly broad. The plateaus are equaly high. But the density graph (a) is less steap in the region next to the support of the plateau than in case (b). Hence, the graph under (b) strictly forbids the step heights $\tau^{-1}S=4.08$ Å.

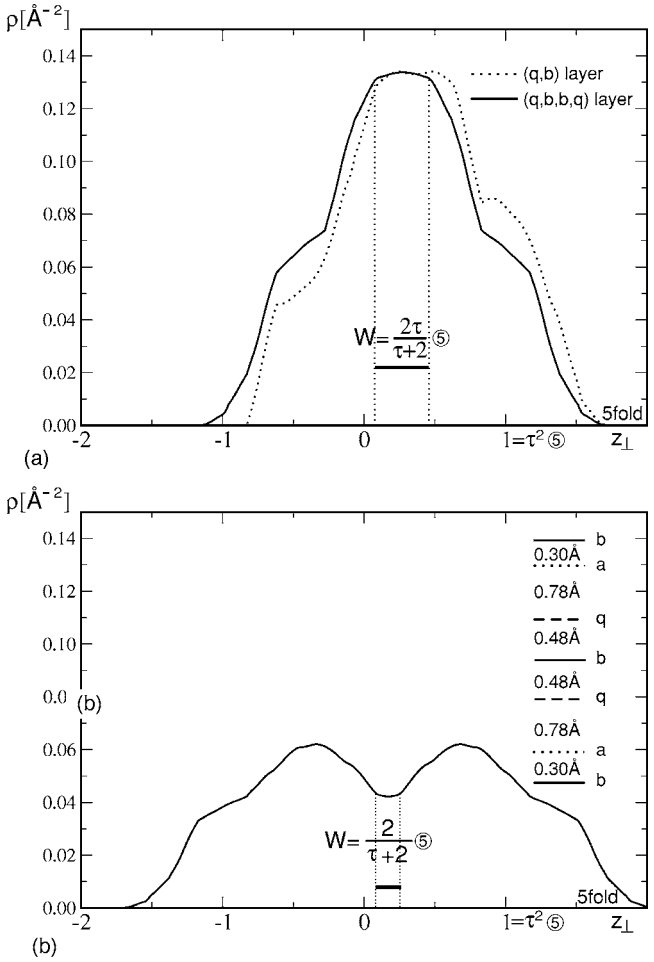

FIG. 4. (a) Density graph $\rho_{5f}(z_\perp)$ of the "thick" fivefold layers (q,b,b,q) (full line). The plateau (maximum density) of the graph defines the terminations. The support of the plateau is $W=[2\tau/(\tau+2)]⑤$ broad. It is compared to the density graph of the 0.48 Å thin, plane-like layer (q,b) (dotted line). The symbol ⑤is the standard distance along a fivefold axis $z_\perp$ in the coding space $\mathbb{E}_\perp$. (b) Density graph of the fivefold layers (b,a,q,b,q,a,b), with spacings as in the image. The bottom of the cavity defines a sequence of the minimum density layers in $\mathcal{M}(\mathcal{T}^{*(2F)})$, situated above a subsequence of the fivefold terminations. The support of the cavity is $W=[2/(\tau+2)]⑤$ broad.

0.48 Å, q plane, 0.78 Å, a plane, 0.78 Å, q plane, 0.48 Å, b plane. The a plane, in the middle, is of negligible density (<0.013 Å^{-2}), if compared to the densities of the surrounding planelike layers in the $[b,q,(a),q,b]$ layer. Hence, neglecting the a plane we can define an effective density as in the case of the (q,b,b,q) layers. The height and the width of the plateaus on the density graphs are of the same size [compare Figs. 3(b) and 3(a)]. But the density graph of the layer (b,q,q,b) [Fig. 3(b)] is steeper in the region next to the support of the plateau than the graph of the layer (q,b,b,q) [Fig. 3(a)], and forbids the terrace height of 4.08 Å to appear. The 4.08 Å terrace height was observed even on the highest annealing temperature 1070 K.[11] That is why we prefer that the support of the plateau of the density graph in case of the (q,b,b,q) atomic layers [see Fig. 4(a)] defines the sequence of fivefold bulk terminations.

Whereas for the thin-layer concept the width of the support of the plateau is approximately $[2\tau^2/(\tau+2)]⑤$ broad [Fig. 4(a)], and consequently[3] encodes the Fibonacci sequence of terrace heights $S=[2\tau/(\tau+2)]⑤=4.08$ Å and $L=\tau S=6.60$ Å $[\tau=(1+\sqrt{5})/2]$, in the "thick layer" concept the width is exactly $[2\tau/(\tau+2)]⑤$ [Fig. 4(a)] and encodes the Fibonacci sequence of by factor τ larger terrace heights, i.e., $L=6.60$ Å and $L+S=\tau L=10.68$ Å. Whereas on the clean surfaces, obtained at lower annealing temperature, even the terrace height $\tau^{-1}S=2.52$ Å appears,[12] on the surfaces obtained at the highest annealing temperature (1070 K), apart S and L also a terrace height $L+S$ appears (Fig. 1 in Ref. 11). The height of the plateau of the graph ρ_{5f} [Fig. 4(a)] defines the densities of the "thick layer" terminations to be 0.134 Å^{-2} (Table I). The fivefold layers intertwining the termina-

TABLE I. Relative and absolute densities of the planes and layer terminations orthogonal to fivefold, twofold, and threefold symmetry axes in $\mathcal{M}(\mathcal{T}^{*(2F)})$ of *i*-AlPdMn. The corresponding data for *i*-AlCuFe are similar.

	Fivefold	Twofold	Threefold
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

tions are of densities not higher than 0.072 Å^{-2} ($\ll$0.134 Å^{-2}). It is also a fact, that the density graphs of the "thin" and the "thick" layers have a strong overlap [Fig. 4(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 $\mathcal{M}(\mathcal{T}^{*(2F)})$ 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 $\mathcal{M}(\mathcal{T}^{*(2F)})$ would be declared as a criterion of a termination to appear below it, as in Ref. 6, the 2.04 Å terrace heights, that were not observed, should appear as well. However in the model $\mathcal{M}(\mathcal{T}^{*(2F)})$ there is a low density fivefold layer (b,a,q,b,q,a,b) [see Fig. 4(b)], 4.08 Å broad. The width of the cavity on the density graph of these layers, $W=[2/(\tau+2)]⑤$, 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 [compare Figs. 4(b) and 4(a)]. Hence, the minimum density layer sequence alone cannot define the terminations, because it does not reproduce even the pairs of large terraces 6.60 Å apart, which were frequently observed.

In the case of twofold terminations, we may replace a single dense twofold terminating atomic *abq* plane[3] by a layer of four 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" twofold layer the peak of $\rho_{2f}(z_\perp)$ is a perfectly flat plateau (Fig. 5). The height of the plateau defines the effective density of terminations to be 0.086 Å^{-2} (Table I). The support of the width of the plateau equals $W=(1/2)②$ (see Fig. 7) and encodes the Fibonacci sequence of twofold terminations with the terrace heights $S=(\tau^2/2)②=6.3$ Å and $L=\tau S=10.2$ Å.

The heights of the larger twofold terraces were measured to be $S=6.2$ Å and $L=9.5$ Å [see Fig. 6(b)] in good agreement with the predicted values. The twofold layers intertwining the terminations are of densities not higher than 0.079 Å^{-2}($<$0.086 Å^{-2}). The pits within the big terraces [see Fig. 6(b)] may be explained by the comparatively large distances between the atomic planes inside of the "thick" terminating layer, 1.5, 2.4, and 3.9 Å (see Fig. 5). These excellently reproduce the measured values 2.4 and 3.6 Å [see Fig. 6(b)].

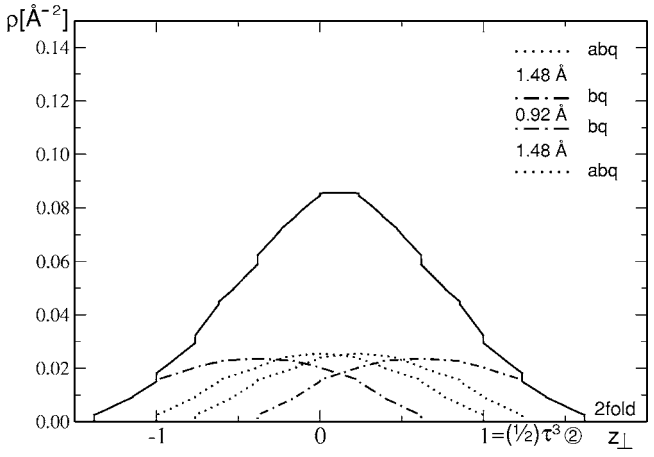

FIG. 5. Density graph $\rho_{2f}(z_\perp)$ of the "thick" twofold layers, with spacings: *abq* plane, 1.48 Å, *bq* plane, 0.92 Å, *bq* plane, 1.48 Å, *abq* plane. The plateau of the graph defines the terminations. The width of the support of the plateau exactly equals ②/2 [see Fig. 7(a)] and defines the Fibonacci sequence of twofold terminations with step heights $S=(\tau^2/2)②=6.3$ and $L=\tau S=10.2$ Å.

In the model $\mathcal{M}(\mathcal{T}^{*(2F)})$ there is a low density twofold layer (bq,bq):0.92 Å gap, *bq* plane, 0.57 Å, *bq* plane, 0.92 Å gap [see Fig. 7(b)]. The support of the cavity, $W=(\tau/2)②$ broad, on the graph of these layers 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 twofold termination. Nevertheless, in the twofold case the minimum density layer sequence *alone* cannot define the terminations, because it predicts by τ^{-1} shorter terrace heights than observed between the large twofold terminations [compare Fig. 7(b) to 7(a)].

The threefold terminations could also be modeled as "thick" layers of atomic planes in $\mathcal{M}(\mathcal{T}^{*(2F)})$, see Table I. But, inspecting the intertwining threefold layers, we see that these are of the densities comparable to the "terminating" ones. We also know that the threefold surfaces facet readily,[4] and some correlated STM measurements (as those in Fig. 6) for the threefold surfaces do not exist so far.

On the STM measurements of fivefold surfaces it is hard to judge whether "thin layer" or "thick layer" terminations best model the surfaces. However, the "thick layer" concept removes the contradiction with respect to Bravais' rule, that some, equally dense layers do not appear on the surfaces, see Ref. 3. Concerning twofold surfaces the "thick layer" concept is evidently better, it treats differently the large terraces compared to the small pits inside.

C. Secondary-electron images

Figure 8(a) shows the pattern of the secondary-electron images (SEI) (Ref. 14) obtained from the clean pentagonal surface of a quasicrystalline $Al_{70}Pd_{20}Mn_{10}$ sample.[8] SEI rep-

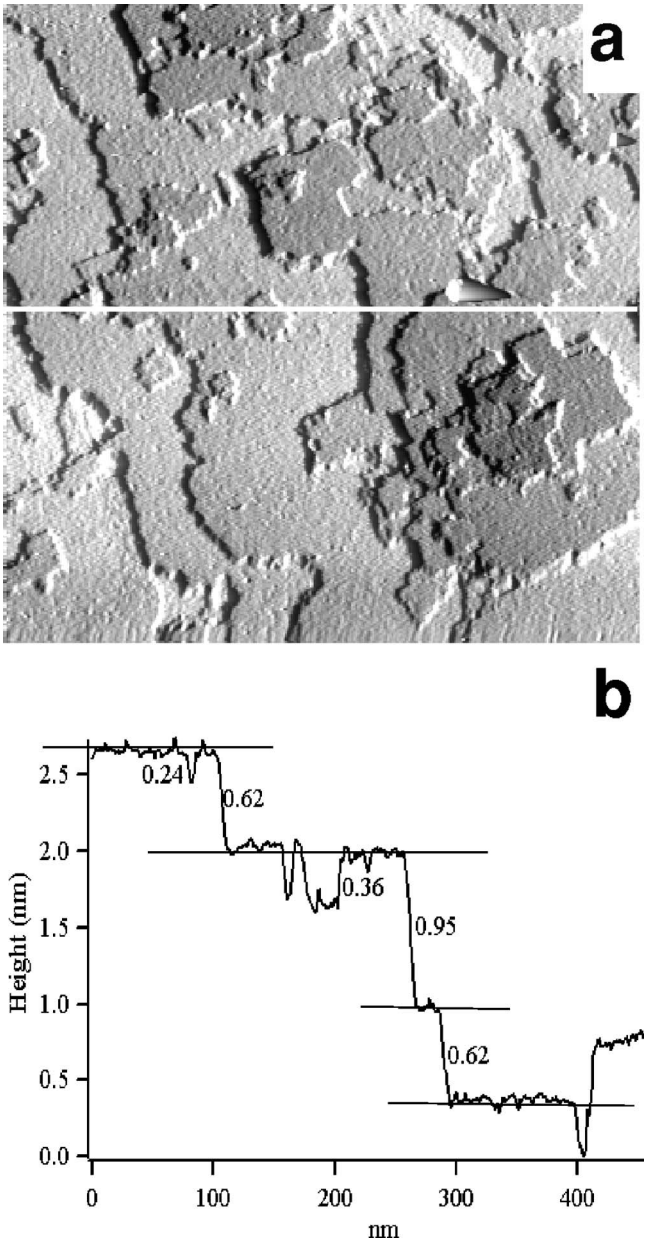

FIG. 6. This figure shows the work of V. Fournée (Refs. 3 and 13): (a) STM image of a twofold terrace-stepped surface of *i*-AlPdMn, size 500×500 nm^2. (b) Correlated measurements, height profile along the white line in (a) with step heights. Note the large terraces with heights 0.62 and 0.95 nm on which are superimposed smaller terraces (pits) with heights 0.24 and 0.36 nm.

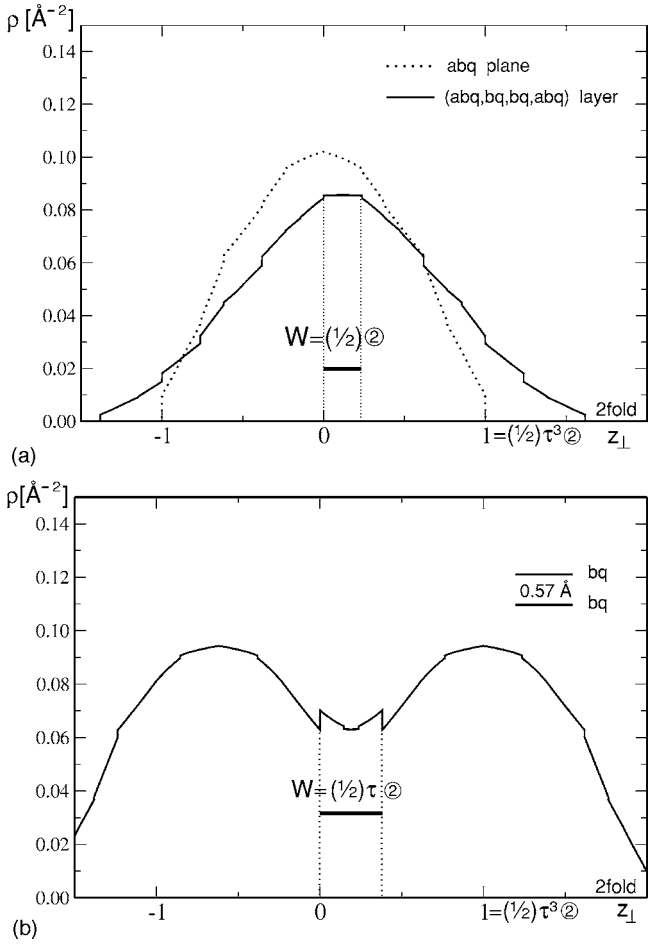

FIG. 7. (a) Density graph $\rho_{2f}(z_\perp)$ of the "thick" twofold layers (full line). The plateau (maximum density) of the graph defines the terminations. The support of the plateau is $W=\frac{1}{2}$② broad. It is compared to the "thin layer" termination (dotted line), which is a single, *abq* plane. The symbol ② is the standard distance along a twofold axis $z_\perp$ in the coding space $\mathbb{E}_\perp$. (b) Density graph of the twofold layer (bq,bq). The cavity defines a sequence of the *minimum density* layers in $\mathcal{M}(\mathcal{T}^{*(2F)})$, of which a *subsequence* is situated above all the twofold terminations. The support of the cavity is $W=(\tau/2)$② broad.

resent an orthogonal projection to the sphere of the symmetry directions below a near-surface region of the sample. Apart from the icosahedral symmetry of the pattern, some groups of bright patches are seen to lie within bands, similar to Kikuchi bands[14] connecting the twofold-, threefold-, and fivefold-symmetry directions. In case of crystals these bands are a direct consequence of well-defined dense *planes* of atoms. The bands observed in a quasicrystal should be also a consequence of dense planes or planelike layers within the quasicrystal, which, according to the secondary-electron SEI pattern, lie perpendicular to the principal directions of the icosahedron. Hence, the pattern in Fig. 8(a) carries an information of the long-range order. We note that there are bands perpendicular to twofold- and fivefold-symmetry directions, but not to threefold-symmetry directions.

A quantum mechanical single-site scattering calculation[14] is a faithful representation of the SEI pattern because it accounts for the wave nature of the secondary electrons. Figure 8(b) illustrates the results of the calculation[15] using the coordinate set of the model $\mathcal{M}(\mathcal{T}^{*(2F)})$. This approximation overestimates the scattering intensity along chains of atoms[14] but suffices for purposes, since our interest is mainly in the presence or absence of bands on the screen. As in case of crystals[14] the band width is inversely proportional to the spacing of crystallographic planes, and the band width is related to the distance of interatomic planes.[14] The observed band widths reveal that the interplanar distances of the highly dense twofold planes are broader than these of the

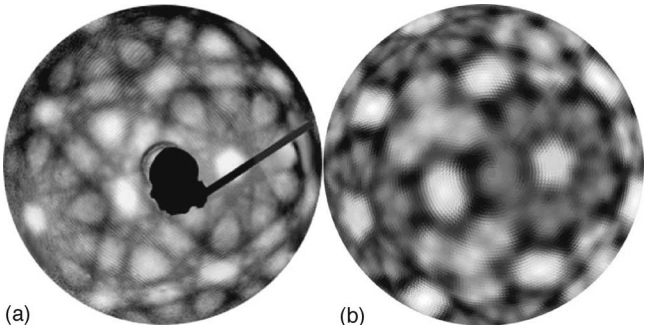

FIG. 8. (a) Secondary-electron pattern (SEI) obtained from the pentagonal surface of a single icosahedral $Al_{70}Pd_{20}Mn_{10}$ quasicrystal. The edge of the screen corresponds to (Ref. 14) $\theta=52°$. (b) Calculated secondary-electron pattern based on the single scattering approximation of electrons (Ref. 15) using model $\mathcal{M}(\mathcal{T}^{*(2F)})$.

fivefold planes/planelike layers by a factor 1.6. In the fivefold case, from the model we predict the distance $d_5=\tau/(\tau+2)$⑤$=2.04$ Å, which is the distance between the highly dense (q,b) and the (b,q) planelike layers in the layers (q,b,b,q) and (b,q,q,b): 2.04 Å=0.48 Å+1.56 Å, see also Ref. 16. In the twofold 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 $d_2=[\tau/(3\sqrt{\tau+2})]$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 Bravais' rule should be valid in quasicrystals as well. The not existing threefold Kikuchi bands are also supporting the model $\mathcal{M}(\mathcal{T}^{*(2F)})$, in which we find that the atoms collected by the threefold planes are almost uniformly distributed among these, without the notable repetitive layers of higher densities.

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