To the model of a decagonal Al-Cu-Co

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Abstract.
It is an approach to the model of a decagonal Al-Cu-Co quasicrystal, reproduced from the data of a scanning transmission electron microscopy (STEM) image. The atomic positions, seen on STEM images should be related to an ideal 2-dimensional pentagonal tiling, obtained by the projection from the 4-dimensional root-lattice.

1. Introduction
A decagonal Al-Cu-Co had been, among other authors, modelled by Burkov [1]. In his model, the stoichiometry is Al\(_{10/5}\)Cu\(_{15}\)Co\(_{15}\), and it is periodic in the 10f/5f direction, with the period of circa 4 Å. Burkov claims that his model is based on the electron microscopy [2] and x-ray diffraction data [3, 4, 5], although Kuo et al. [3, 4, 5] consider Al\(_{25}\)Cu\(_{20}\)Co\(_{15}\) with periodicity of circa 8 Å.

A variant of the Burkov model was latter founded over the pentagonal tiling [8] has as the prototiles two golden triangles. Both golden triangles are isosceles, triangles having two sides equal. The isosceles triangle, that we label by the letter ‘D’, has the base side (edge) of length ➁, and two edges of an equal length ➁. The standard length ➁ is along a 2f direction. Another isosceles triangle, labelled by the letter ‘d’ has the base edge of length ➁.

In what follows we will address to the STEM image done along the c-axis, perpendicular to the quasiperiodic planes. This image is presented in Figs 3 and 4 of Ref [7]. Al\(_{64}\)Cu\(_{22}\)Co\(_{14}\) [7] are on a decagonal phase with the period of circa 4 Å, as by Burkov. In this paper the tiling ⃔(A4) will be put over the STEM image from Ref [7], and the result will be compared to the way how it was previously done in the Burkov model.

2. The triangular tiling over the STEM image of Al\(_{64}\)Cu\(_{22}\)Co\(_{14}\)
The pentagonal tiling ⃔(A4) [8] has as the prototiles two golden triangles. Both golden triangles are isosceles, triangles having two sides equal. The isosceles triangle, that we label by the letter ‘D’, has the base side (edge) of length ⃔, and two edges of an equal length ⃔. The standard length ⃔ is along a 2f direction. Another isosceles triangle, labelled by the letter ‘d’ has the base edge of length ⃔, and two edges of an equal length ⃔.

In what follows we will address to the STEM image done along the c-axis, perpendicular to the quasiperiodic planes. This image is presented in Figs 3 and 4 of Ref [7]. In Ref [7] Al\(_{64}\)Cu\(_{22}\)Co\(_{14}\) is identified as a decagonal quasicrystal, periodic along the c-axis, and the length of the period is estimated to be circa 4.00 Å. The strong shining spots are identified on Fig 4 in Ref [7] as the transition metals, and the less shining, or almost not seen spots are interpreted as Al positions. In this paper we will reduce our attention to the strongly shining spots, and among these, to the spots forming local configurations of the pentagonal symmetry.
Let us have a look on STEM image on Fig 3a of Ref [7]. Among the shining spots there appear two smallest local configurations with the pentagonal symmetry, a pentagram (five pointed star) \( S \), and the pentagon \( P \). We mark the pentagram \( S \) in red and the pentagon \( P \) in dark blue, see Fig 1. On the STEM image a patch of the \( \mathcal{T}^{*}(A_4) \) tiling is drown with light blue edges, all along the 2f directions. We see that prototiles, scaled from above defined \( D \) and \( d \) can have two different decorations by the shining spots (TM positions) depending on their orientation with respect to the pentagram \( S \). For the reason we label these by \( D_1 \) and \( D_2 \) and by \( d_1 \) and \( d_2 \), see Fig 1.

By the white broken line is drown a plane orthogonal to the 5f/10f image plane, such that either to the left or to the right hand side of the plane an ideal tiling patch is seen. It is evident from the fact that the single vertex configuration of the tiling that appears on the broken line is not an allowed vertex configuration in the tiling \( \tilde{\mathcal{T}}^{*}(A_4) \) [8].

Let us introduce the scale on the tiling. The long edge of the golden triangles congruent to \( D \) and \( d \) corresponds to the \( \tau^3 \odot \), with \( \odot \) being the standard length along a 2f direction. Note that the prototiles of by \( \tau^2 \) augmented tiling \( \mathcal{T}^{*}(A_4) \) are labeled by the same labels, as the standard tiling \( \mathcal{T}^{*}(A_4) \), introduced at the beginning. The long edge of the tiling, compared to the 1nm unit on the STEM image is \( \tau^3 \odot = 19.51 \text{Å} \). The value is very close to 19, 6Å, the length of the long edge estimated in the Burkov model [1]. The edge length of the pentagon \( P \), drown in dark blue in Fig 1 is then \( \tau^{-1} \odot = 2.85 \text{Å} \), whereas an ‘arm’ of the pentagram (five pointed star) \( S \), marked in Fig 1 in red is \( \odot 2\tau/(\tau + 2) = 3.92 \text{Å} \), with \( \odot \) being the standard length along an icosahedral 5f direction. Hence, we conclude that the length of the standard basis vectors in the high dimensional lattice \( \mathbb{Z}_5 \) is \( |e_i| = 6.19 \text{Å} \) \((i = 1, 2, \ldots, 5)\). Projected into the standard length [5] onto the quasiperiodic plane, [5] := \( \odot 2\tau/(\tau + 2) = 3.92 \text{Å} \), or circa 0.4nm. It is labelled in red on the images.

Let us mark the local configurations on which the vertices of the tiling in Fig 1 are fixed. It turns out that these are the pentagrams \( S \), see Fig 2. Moreover, all the \( S \) configurations from the STEM image are

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**Figure 1.** Over the STEM image of Al_{0.4}Cu_{0.2}Co_{0.14} from Ref [7] the tiling \( \mathcal{T}^{*}(A_4) \) by two golden triangles is drown. The four decorated prototiles \( D_1 \), \( D_2 \), \( d_1 \) and \( d_2 \) are marked. The variants ‘1’ or ‘2’ of decorations are particularly oriented with respect to the pentagram (five pointed star) \( S \), marked in red. The length of the pentagram-arm is circa 0.4 nm. Also the pentagon \( P \) is marked in dark blue. The length of the pentagon-edge is circa 0.6 nm.
the vertices of the tiling $\mathcal{T}^s(A_4)$.

Figure 2. All the $S$ configurations (pentagrams, marked in red) from the STEM image of Al$_6$Cu$_{22}$Co$_{14}$ are the vertices of the tiling $\mathcal{T}^s(A_4)$.

Figure 3. By full lines in light blue is presented a patch of the tiling $\mathcal{T}^s(A_4)$ with the vertices on some of the $P$ configurations over the STEM image of Al$_6$Cu$_{22}$Co$_{14}$. If the dashed light blue lines are added, there appears by $\tau^{-1}$ deflated tiling, though with not all the vertices on the $P$ configurations.

According to Fig 4 in Ref [7], the pentagon $P$ has at the vertices large shining spots, identified as the TM positions. On a pentagon of the same size, rotated by $36^\circ$, the smaller spots are interpreted as Al
positions. The union of these two pentagons is a decagon. If one compares Figs 1 and 2 of the present paper to the Fig 3 in Ref [6], a patch of the Burkov model, one finds in Fig 3 in Ref [6] decagons of the same size, as a union of the mentioned two pentagons, but with the TMs placed on both pentagons. On a STEM image such a configuration should appear as a strong shining decagon. These decagons are centered on the vertices of the tiling $T_{\tau}(A_4)$, see Fig 3 in Ref [6]. Let us try to put a tiling $T_{\tau}(A_4)$ on the STEM image of Al$_{65}$Cu$_{15}$Co$_{20}$, such that all vertices are on the pentagons $P$, see Fig 3 in the present paper. It turns out, that the tiling $T_{\tau}(A_4)$, fulfilling this condition is augmented by factor $\tau$, compared to the tiling with the vertices on pentagons $S$, as in Fig 2. If the first step of deflation is performed on Fig 3, one ends up with the tiling on the same scale as in Figs 1 and 2, but the patch of the tiling does not have all the vertices centered at the pentagons $P$.

Let us consider the high-resolution electron microscopy image of Al$_{65}$Cu$_{15}$Co$_{20}$ presented in Fig 3(a) of Ref [2]. The pentagrams $S$ are not seen on the image, but some decagonal/pentagonal configurations of the same size as the pentagons $P$ of Al$_{65}$Cu$_{15}$Co$_{20}$ (see Fig 1) are clearly identified. On the image in Fig 3(a) of Ref [2] the “Penrose 1” tiling (P1) is put on these pentagons/decagons $P$ as the vertices. The edge length of P1 is circa 20 Å. It is evident that the tiling P1 with the edge length scaled by $\tau^{-1}$ can not be supported by the $P$ configurations at all the vertices. In Fig 2(c) of Ref [7] a P1 tiling with the smallest possible edge is plotted over the 5f image of Al$_{65}$Cu$_{15}$Co$_{20}$ such that all the vertices of the tiling P1 are on configurations $P$. It turns out that the edge length is circa 20 Å, as well. Through the inspection it can be seen that the quasilattices of the $P$ configurations in both decagonal phases could probably be considered as equivalent. Hence, in both cases the underlying triangular tiling $T_{\tau}(A_4)$ by the smallest possible tiles with all the vertices on pentagons $P$ has the short edge of 20 Å, as the tiles drawn in full lines in Fig 3. For the relation of the $T_{\tau}(A_4)$ to the P1 tiling see Ref [9]. The conclusion is that the frequency of the pentagons/decagons $P$ is overestimated in the Burkov model.

3. Outlook
A lattice point $x$ of the reciprocal lattice $A_4^R$ can be written in the basis $\{a_i = e_i - \frac{1}{2} e_5, i = 1, 2, \ldots, 5, s = e_1 + e_2 + \ldots + e_5\}$ as $x = \sum_{i=1}^{5} n_i a_i$ ($n_i$ are integers). With respect to the translations of the $A_4$ lattice this set splits into 5 classes: $r(q^R) := \sum_{i=1}^{5} n_i \mod 5$. The function $r(q^R)$ takes five possible values: 0, 1, 2, 3 and 4. One of these classes labels the lattice points in the lattice $A_4$, the further 4 classes are the holes of the lattice $A_4$. Using the single cluster from Fig 4 in Ref [7] and distributing it among the prototiles $D_1$, $D_2$, $d_1$, and $d_2$ one easily classifies the shining spots of the STEM image into five classes (presented at Aperiodic’09). But, in the overlap of two such clusters there appear some too short interatomic distances. The way out of the problem will be in changing somewhat the atomic positions on a periphery of the suggested cluster.

Another problem with the model will be to fix accurately the Al positions. An STM image of the clean 5f surface, with probably high concentration of Al atoms could be useful.

And finally, for the distribution of the planar images of the atomic positions into different planes orthogonal to the c (5f) axis within the period, a STEM image in the 2f direction is needed.

4. References
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