

# Cluster environments in a twelve-fold packing model of icosahedral quasicrystals

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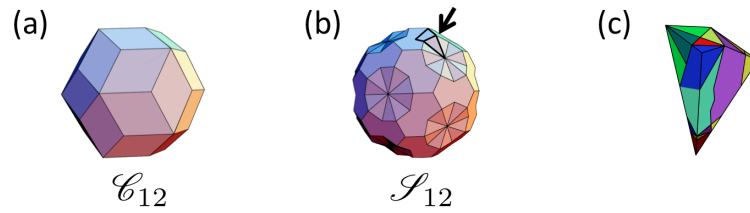
**Abstract.** The shapes of the occupation domains that correspond to the respective local environments of the clusters within a 12-fold packing model of icosahedral quasicrystals (iQCs) have been derived for the first time. The frequencies of appearance of the local environments of the clusters have also been calculated based on the exact volumes. The present results validate the frequencies obtained by a previous study using a statistical approach. Application of the 12-fold packing model to the F-type Al-based iQCs is discussed briefly.

## 1. Introduction

The twelve-fold (12-fold) packing vertices is a subset of the 12-fold vertices that have all twelve possible edges radiating from them along 5-fold directions out of the vertices of a three-dimensional Ammann-Kramer-Neri (3D-AKN) tiling (or a 3D generalisation of Penrose tiling) [1, 2]. The 12-fold packing vertices are characterised by the shortest distance  $c$  between a pair of the vertices along 3-fold directions ( $c$ -link), and the next-shortest distance  $b$  along 2-fold directions ( $b$ -link). Their distances are related to  $a$ , the edge length of 3D-AKN tiling, as  $b = a(4 + 8/\sqrt{5})^{1/2}$  for  $b$ -links and  $c = b(\sqrt{3}/2)$  for  $c$ -links. Short  $a$ -links with length  $a$  that exist in the 12-fold vertices along 5-fold directions are eliminated. The geometries of the 12-fold packing vertices were studied in detail by Henley in the context of sphere packing problem as a theoretical structure model of icosahedral quasicrystals (iQCs) [2, 3]. A successful structural description for the Yb-Cd iQC has been given as a 6D structure model, where Tsai-type clusters are arranged at the 12-fold packing vertices generated by a particular shape of occupation domain (Fig. 1(b)) [4, 5]. The geometrical properties of iQCs model based on the 12-fold packing vertices was discussed in a literature [6].

The model of the Yb-Cd iQC is a representative model based on the 12-fold packing vertices of a 3D-AKN tiling, or 12-fold packing model for short [5, 6]. It consists of three building units: rhombic triacontahedron (RT), acute rhombohedron (AR), and obtuse rhombohedron (OR). By choosing an appropriate length for the edges for an underlying 3D-AKN tiling and by giving appropriate atomic decorations to the three building units, a complete atomic structure model for an iQC can be constructed. The binary Yb-Cd iQC model is the case that unique atomic decorations can be given to the building units [5, 6]. According to the previous studies, the 12-fold packing vertices have coordination numbers in the range from 7 to 12 [2, 6]. Frequencies





**Figure 1.** (a) The occupation domain  $\mathcal{C}_{12}$  for the 12-fold vertices of a 3D-AKN tiling. (b) The archetype occupation domain  $\mathcal{S}_{12}$  for the 12-fold packing vertices, and (c) its asymmetric part (arrowed part in (b)). The tessellation indicates the sectors that generate different vertex environments (see text and Fig. 2).

for 18 different vertex (or cluster) environments were evaluated numerically for the specific occupation domain (Fig. 1(b)) [6]. However, the corresponding shape of the occupation domain for each vertex environment is unknown. The aim of this work is to present the shapes of the occupation domains for each cluster environment for the specific occupation domain (Fig. 1(b)). This information will be useful when one consider an extended model of the Yb-Cd iQC including local chemistry for ternary iQCs or a similar model with different cluster types, such as Bergman or Mackay types or both.

## 2. Occupation domains

We recall the basic relationships between occupation domains defined in the internal space (or perpendicular space) within the section (or cut) method [1, 2, 7]. Consider an 3D-AKN tiling with edges of length  $a$ . The set of the vertices is generated by using an occupation domain,  $\mathcal{C}$ , with RT shape with edges of length  $a$  [1, 2]. The set of 12-fold vertices is a subset of those of the 3D-AKN tiling. The corresponding occupation domain,  $\mathcal{C}_{12}$  (Fig. 1(a)), comes from the central part of  $\mathcal{C}$ , which also has RT shape yet with the edges of length  $a/\tau^2$  [2]. Here  $\tau \equiv (1 + \sqrt{5})/2$  is the golden mean. Since the 12-fold vertices include pairs of the vertices having the length  $a$  along 5-fold directions ( $a$ -links), one vertex from each pair has to be eliminated. The simplest realization of it is  $\mathcal{S}_{12}$  (Fig. 1(b)). This occupation domain was utilised as an archetype occupation domain for the Yb-Cd iQC model [5].

## 3. Cluster environments and the shapes of occupation domains

The cluster local environment in a 12-fold packing model is distinguished by the numbers of  $b$ - and  $c$ -links and the configuration of them [2, 3, 6]. We use a similar notation that used in a previous study, such as  $(\text{CN}, Z_b, Z_c)$  and its corresponding representative 6D vector, where CN is a coordination number that is the sum of the number of  $b$ -links,  $Z_b$ , and that of  $c$ -links,  $Z_c$  [6]. For the sake of simplicity, the edge length for  $\mathcal{C}_{12}$  is normalised as unity, namely  $a/\tau^2 = 1$  in the following calculations.

In the present study, the exact shape of the sector corresponding to each local environment in the asymmetric part of  $\mathcal{S}_{12}$  (Fig. 1(c)) was obtained by two steps. First, the shape of a sector was obtained by a program using CGAL: Computational Geometry Algorithms Library [8]. Second, the coordinates of the vertices for each sector were expressed in the unit of  $(2 + \tau)^{-1/2}$  and transformed them into error free formulae using  $(\alpha + \beta\tau)/\gamma$ , where  $\alpha, \beta$  are any integers, and  $\gamma$  is a positive integer. The volume of each sector was calculated based on the vertices expressed with those error free formulae. The results are listed in table 1. The volume of the asymmetric part of  $\mathcal{S}_{12}$  (Fig. 1(c)) is given as  $(-37 + 23\tau)/6$ . The frequency of appearance for each local environment is thus obtained simply as a relative ratio of the volumes. The values are given down to six decimal places. The present results validate the frequencies obtained by a previous study using a statistical approach [6].

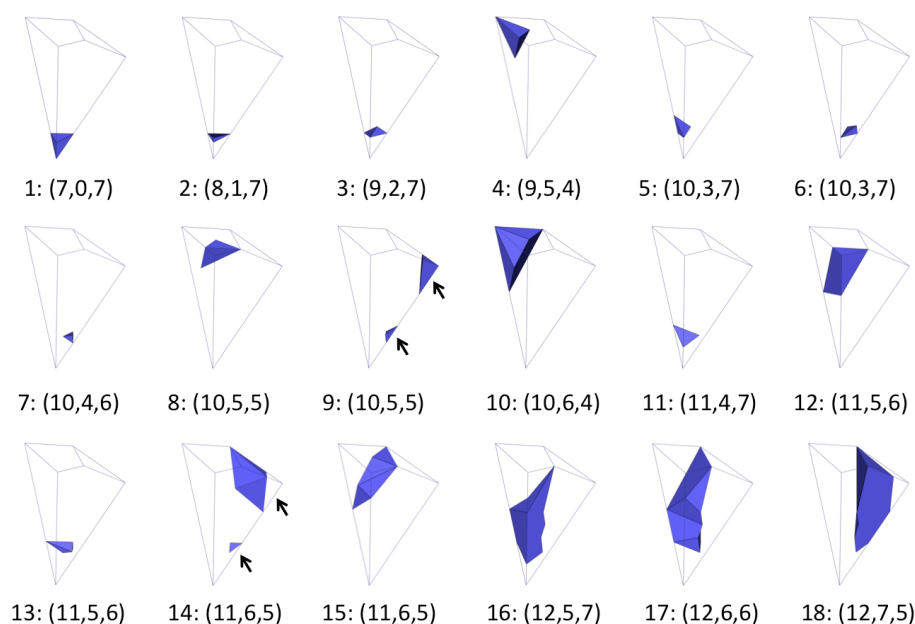
The sectors that correspond to the respective local environments are shown in Fig. 2. Their shapes in the asymmetric part of  $\mathcal{S}_{12}$  appear as tetrahedron, pentahedron, hexahedron, heptahedron, octahedron, hendecahedron, or dodecahedron. It should be noted that the sector of No.9 with (10,5,5) configuration and that of No.14 with (11,6,5) configuration consist of two disconnected parts, as indicated by arrows.

**Table 1.** Local environments in the twelve-fold packing vertices by  $\mathcal{S}_{12}$  of the 3D-AKN tiling. The volume of the sector in the asymmetric part is presented in the unit of  $(2+\tau)^{-1/2}$ .

No.	CN	$Z_b$	$Z_c$	6D vector	Frequency (%)	Volume of the sector
1	7	0	7	(2 0 0 0 0 -1)	1.445942...	(233-144 $\tau$ )/6
2	8	1	7	(3 1 1 0 -2 0)	0.341340...	(-987+610 $\tau$ )/6
3	9	2	7	(4 1 1 0 0 -1)	0.421920...	(1597-987 $\tau$ )/3
4	9	5	4	(2 1 1 -2 0 -2)	1.787282...	(-377+233 $\tau$ )/3
5	10	3	7	(3 1 1 -1 -1 -2)	0.682681...	(-987+610 $\tau$ )/3
6	10	3	7	(5 1 0 1 0 0)	0.377376...	(-7142+4414 $\tau$ )/15
7	10	4	6	(5 1 0 0 0 0)	0.140640...	(1597-987 $\tau$ )/9
8	10	5	5	(3 1 0 -1 0 -2)	1.104601...	(610-377 $\tau$ )/3
9	10	5	5	(5 0 0 0 0 0)	1.642054...	(-2804+1733 $\tau$ )/90
10	10	6	4	(3 0 0 -1 0 -2)	10.46293...	(322-199 $\tau$ )/3
11	11	4	7	(4 1 0 -1 0 -1)	0.610608...	(4414-2728 $\tau$ )/15
12	11	5	6	(3 0 0 0 0 -3)	5.161148...	(-631+390 $\tau$ )/18
13	11	5	6	(4 0 0 -1 0 -1)	0.411660...	(-1364+843 $\tau$ )/18
14	11	6	5	(4 0 0 -1 -1 -1)	5.129700...	(416-257 $\tau$ )/90
15	11	6	5	(3 1 0 0 0 -3)	7.430412...	(-1330+822 $\tau$ )/9
16	12	5	7	(3 0 -1 -1 0 -2)	13.582381...	(678-419 $\tau$ )/9
17	12	6	6	(3 0 -1 -1 -1 -2)	24.398671...	(-3857+2384 $\tau$ )/45
18	12	7	5	(3 -1 -1 -1 -1 -2)	24.868639...	(280-173 $\tau$ )/9

#### 4. Discussion

A cubic approximant crystal that corresponds to F-type Al-based iQCs in Al-Pd-Cr-Fe system has been found recently [9]. The structure can be interpreted as a  $2 \times 2 \times 2$  superstructure of Henley's cubic  $3/2$  packing, and that the parity of each vertex determines the kind of associated cluster, namely, pseudo-Mackay-type or mini-Bergman-type [3, 9]. Note also that the proper lattice constant estimated for F-type iQCs is  $a \approx 0.56$  nm, which is  $\tau^{-1}$  times smaller than that adopted by previous iQC models [10, 11]. It is known that a set of 12-fold packing vertices can be divided into even and odd parity vertices; the  $c$ -links have opposite parities, while the  $b$ -links have the same parities [2]. This discrimination results in F-type order with doubled unit cell in size in 6D space. By decorating each vertex with one of these two types of clusters according to the parity, a 6D model for F-type Al-based iQCs, such as i-Al-Pd-Mn and i-Al-Cu-Fe, can be constructed [12]. The pseudo-Mackay-type cluster is known to contain around 8 atoms, excluding a central atom, in the core of the cluster [13]. The knowledge of the local environment of the clusters is of help in understanding the number and the arrangement of those atoms geometrically, since the pseudo-Mackay-type cluster and mini-Bergman-type cluster heavily overlap with  $c$ -link, and the  $c$ -links are responsible for the formation of a pseudo-Mackay-type cluster [9, 12].



**Figure 2.** The sectors of the occupation domains that correspond to the respective local environments of the 12-fold packing vertices generated by  $\mathcal{S}_{12}$ .

## 5. Conclusion

In this paper we have derived the shape of the occupation domains that correspond to the particular local environments of clusters within a 12-fold packing model of iQCs. The frequencies of appearance of the particular local environments of clusters have also been calculated using the exact volumes. The present results validate the frequencies obtained by a previous study using a statistical approach [6]. Also the results will be useful when one consider an extended model of the Yb-Cd iQC including local chemistry for ternary iQCs or a similar model with different cluster types, such as Bergman-type or Mackay-type or both.

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