International Journal of Applied Nanotechnology Research
Volume 4 • Issue 1 • January-June 2019

Higher Dimensions of Clusters of Intermetallic Compounds:
Dimensions of Metallic Nanoclusters

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ABSTRACT

The author has previously proven that diffraction pattern of intermetallic compounds (quasicrystals) have translational symmetry in the space of higher dimension. In this paper, it is proved that the metallic nanoclusters also have a higher dimension. The internal geometry of clusters was investigated. General expressions for calculating the dimension of clusters is obtained, from which it follows that the dimension of metallic nanoclusters increases linearly with increasing number of cluster shells. The dimensions of many experimentally known metallic nanoclusters are determined. It is shown that these clusters, which are usually considered to be three - dimensional, have a higher dimension. The Euler-Poincaré equation was used, the internal geometry of clusters was investigated.

KEYWORDS

Cluster, Dimension, Edge, Face, Icosahedron, Polytope, Vertices

INTRODUCTION

Currently, a large amount of scientific literature is devoted to the study of nano objects (Gubin, 2019; Haberland, 1994; Gusev, & Rempel, 2000; Suzdalev, 2005). A systematic study of the geometry of the structures of chemical compounds (Zhizhin, 2017, 2018) showed that almost all elements of the periodic system form molecules of higher dimension. It is natural to assume that clusters, as larger than formation molecules, including a large number of atoms, can have a higher dimension. However, until recently, clusters as three-dimensional objects (Lord, Mackay, & Ranganathan, 2006; Pauling, 1960). There are abstract methods for describing clusters, strictly speaking, not related to specific chemical compounds (Diudea & Nagy, 2007; Ashrafi, Cataldo, Iraumanesh, & Ori, 2013). In these works, proceeding from the well - known three - dimensional polyhedrons of Plato and Archimedes, they are transformed by various operations: construction of a polyhedron by the midpoints of edges, truncation, construction of a dual polyhedron, adding vertices of a polyhedron, etc. At the same time, such transformations are in no way connected with real chemical compounds. In addition, consideration of the transformed bodies is carried out in a certain abstract space, as if "forgetting" about the real dimension of chemical compounds (MacMullen, & Schulte, 2002). This cluster research direction is most clearly formulated in a generalizing monograph of Diudea (2018). In the preface to it, it is directly emphasized that the cluster models built in it are not associated with

DOI: 10.4018/IJANR.2019010102

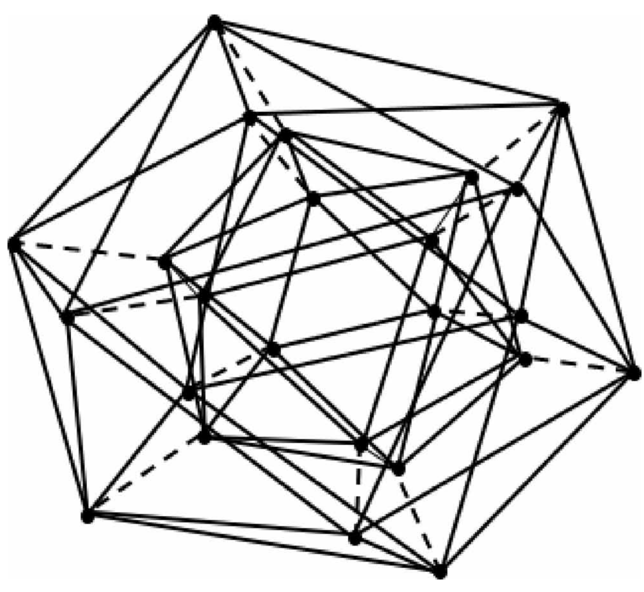
specific crystallographic objects: real crystals, networks, and quasicrystals. This paper discusses clusters of real chemical compounds. Moreover, in this work, consideration of clusters is limited to a special type of chemical compounds - intermetallic compounds, since the study of intermetallic compounds has had a significant impact on the development of scientific views in recent decades. In particular, the discovery of so-called quasicrystals is associated with intermetallic compounds, i.e. crystals supposedly devoid of translational symmetry (Shechtman, Blech, Gratias, & Cahn, 1984). Although it was later shown that quasicrystals have translational symmetry, but in the space of higher dimension (Shevchenko, Zhizhin, & Mackay, 2013 a, b; Zhizhin, 2014c; Zhizhin, & Diudea, 2017).

Clusters of Mackay

Mackay's cluster consists of two icosahedrons of different sizes with a common center (Mackay, 1962). A larger icosahedron is obtained by attaching a number of tetrahedrons and octahedrons to the surface of the smaller icosahedron. However, to determine the dimension of Mackay's cluster, only the result of this connection is important - the formation of a larger icosahedron. Moreover, each vertex of the larger icosahedron is located on a certain line passing through the common center of the icosahedrons. On the same line is located one of the vertices of the smaller icosahedron (Lord et al., 2006). In all vertices of each icosahedron, one atom is located. In addition, there is one more atom in the middle of each edge. Since the icosahedron has 12 vertices and 30 edges, it turns out that Mackay's cluster has 54 atoms (Figure 1).

In this figure, the atoms in the midpoints of the edges of the larger icosahedron are not shown, since in determining the dimension the atoms located on the linear portions of the edges do not matter. Connect the edges of the vertices of both icosahedra lying on the same line passing through the common center of the icosahedrons (dotted lines in Figure 1). The icosahedra are arranged symmetrically with respect to a common center and each other. Therefore, the straight line that leaves the common center and passes through the vertex of one of the icosahedra necessarily passes through the corresponding vertex of the other icosahedron. This shows that the space between the icosahedrons is completely filled with triangular prisms, the bases of which are the triangular faces of the smaller and larger icosahedrons.

Figure 1. The cluster of Mackay



These prisms are adjacent to each other along flat quadrilateral side faces. The number of these prisms is equal to the number of triangular faces of the icosahedron, i.e., 20. To determine the dimension of the construction of two icosahedra with a common center, between which there are 20 triangular prisms, make use of the Euler – Poincaré formula (Poincaré, 1895):

$$\sum_{i=0}^{d-1}(-1)^i f_i(P) = 1 + (-1)^{d-1} \quad (1)$$

In (1) $f_i(P)$ is the number of faces with dimension *i* in polytope *P* with dimension *d*.
For a given design, we have:

$$f_0 = 2\cdot 12 = 24, f_1 = 2\cdot 30 + 12 = 72, f_2 = 2\cdot 20 + 30 = 70, f_3 = 20 + 2 = 22$$

Substituting these values in the Equation (1), we obtain 24 – 72 + 70 – 22 = 0. This proves that the dimension of Mackay's cluster with two only icosahedral shells is 4.
To the first as well the second icosahedron the tetrahedrons and octahedrons can be attached and a third icosahedral shell can be obtained. This process can be continued.

Theorem 1: The dimension *d* of a cluster of *n* - icosahedrons with a common center is 2 + *n*.
Proof: If a cluster consists of three shells of an icosahedron with a common center, then:

$$f_0 = 3\cdot 12 = 36, f_1 = 3\cdot 30 + 2\cdot 12 = 114, f_2 = 3\cdot 20 + 2\cdot 30 = 120, f_3 = 2\cdot 20 + 3 = 43$$

The number of four - dimensional figures in this case is equal to $f_4 = C_3^2 = 3.$ Substituting these values in the Equation (1), we have 36 – 114 + 120 – 43 + 3 = 2. This proves that the dimension of Mackay's cluster with three icosahedral shells is *d* = 5.
If a cluster consists of four shells of an icosahedron with a common center, then:

$$f_0 = 4\cdot 12 = 48, f_1 = 4\cdot 30 + 3\cdot 12 = 156, f_2 = 4\cdot 20 + 3\cdot 30 = 170, f_3 = 3\cdot 20 + 4 = 64$$

The number of four - dimensional figures in this case is equal to $f_4 = C_4^2 = 6.$ The number of five - dimensional figures in this case is equal to $f_5 = C_4^3 = 4.$ Substituting these values in the Equation (1), we have 48 – 156 + 170 – 64 + 6 - 4 = 0. This proves that the dimension of Mackay's cluster with four icosahedral shells is *d* = 6. If a cluster consists of five shells of an icosahedron with a common center, then:

$$f_0 = 5\cdot 12 = 60, f_1 = 5\cdot 30 + 4\cdot 12 = 198, f_2 = 5\cdot 20 + 4\cdot 30 = 220, f_3 = 4\cdot 20 + 5 = 85$$

The number of four - dimensional figures in this case is equal to $f_4 = C_5^2 = 10.$ The number of five-dimensional figures in this case is equal to $f_5 = C_5^3 = 10.$ The number of six – dimensional figures is equal to $f_6 = C_5^4 = 5.$ Substituting these values in the Equation (1), we find 60 – 198 + 220 – 85 +10 – 10 + 5 = 2. This proves that the dimension of Mackay's cluster with five icosahedral shells is *d* = 7. These constructions can be continued. However, it is now possible to write general expressions for the numbers of elements of different dimensions in a cluster with an arbitrary number *n* of shells of icosahedra and to give a formula for calculating its dimension. So, in the *n* - shell cluster of icosahedrons, we have:

$$f_0 = n \cdot 12, f_1 = n \cdot 30 + (n-1) \cdot 12, f_2 = n \cdot 20 + (n-1) \cdot 30, f_3 = (n-1) \cdot 20 + n,\\ f_4 = C_n^2, f_5 = C_n^3, \ldots, f_{n+1} = C_n^{n-1}. \quad (2)$$

If substitute these values into Equation (1) and opening the brackets you can see that in this case the left side of the Euler – Poincaré Equation (1) takes the form:

$$\sum_{i=0}^{d-1} (-1)^i f_i(P) = 2 - n + \sum_{k=2}^{n-1} C_n^k (-1)^k \quad (3)$$

To calculate the sum on the right side of Equation (3), we use the well-known expression for the alternating series of combinations (Vilenkin, 1969):

$$C_n^0 - C_n^1 + C_n^2 - \ldots + (-1)^n C_n^n = 0. \quad (4)$$

From the series (4), taking into account the equalities $C_n^0 = C_n^n = 1, C_n^1 = n$, it follows that when *n* is even the sum $\sum_{k=2}^{n-1} C_n^k (-1)^k$ in the right side of Equation (3) is *n* – 2 while *n* is odd the sum is equal to *n*. Therefore, the right side of Equation (3) coincides with the right side of Equation (1). This proves that the figures in question are closed convex polytopes and they satisfy the Euler – Poincaré equation. At the same time, from Equation (2), since $f_{n+2} = C_n^n = 1$, it follows that the dimension *d* of a cluster of *n* - icosahedrons with a common center is equal to *n* + 2. Q.E.D.

Thus, it is proved that the dimension of a cluster of *n* icosahedral shells with a common center increases linearly with the number of icosahedral shells. The total number of atoms in a cluster, including the n^{th} layer, is $n(10n^2 + 15n + 11) / 3$ (Lord et al., 2006).

Clusters of γ – Brass

The structure of γ - brass was described as early as 1926 in the concept of a lattice of cubic cells (Bradley, &Thewlis, 1926). Pauling (1960) while considering the structure of γ - brass, noticed that this structure is icosahedral (Pauling, 1960). Nyman & Anderson (1979) described the alloy Mn_5Si_3, Th_6Mn_{23} and γ - brass as a 26 - atomic cluster of identical balls, although it should be noted that atoms are not identical balls. First, the electron orbitals of atoms in the outer layer have a complex shape, very far from the shape of a ball, especially for transition metals. Secondly, different metals are used in the alloys, they are not identical.

Theorem 2: A γ - brass cluster has the dimension *d* = 4 + 3*n*, where *n* is the number of cluster shells (*n* = 0, 1, 2, …). The cluster is a *d* - cross - polytope and the number of elements of the dimension *i* included in the cluster is determined by the ratio $f_i(d) = 2^{1+i} C_d^{d-1-i}$.

Proof: Alloys of γ - brass, as well as other intermetallic alloys, are conveniently considered using tetrahedrons (Lord et al., 2008). Place four atoms at the vertices of the 1234 tetrahedron.

Then on each flat face of the tetrahedron 1234 one set up another tetrahedrons (Figure 2). (Elements of any dimension in a polytope are called faces.)

Next, the figure appears including 8 atoms (vertices 1 - 8). Connect the vertices 5, 6, 7, 8 of edges. They also form a tetrahedron. As a result, the resulting figure (Figure 3) is a 4 - cross - polytope (Zhizhin, 2018).

In this polytope, in addition to 8 vertices, there are 24 edges, 32 flat triangular faces, and 16 tetrahedrons. Each vertex has no edge connection to some other (opposite) vertex. These unconnected vertices form pairs 1 – 7, 2 – 8, 3 – 5, 4 – 6. This pairs can to place vertically:

1 2 3 4
7 8 5 6

Each vertex in the top row the numbers does not have a connection with the vertex in the bottom row, just below this vertex. This polytope has dimension 4. Upon further joining of the tetrahedrons to the edges of the original tetrahedron 1234 (two tetrahedrons to the edge), a figure is formed containing 14 vertices. Each newly formed vertex is located opposite one of the edges of the tetrahedron 1234.

Figure 2. The tetrahedron with tetrahedrons on its faces

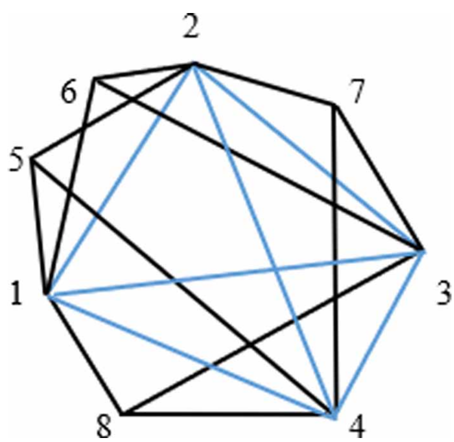
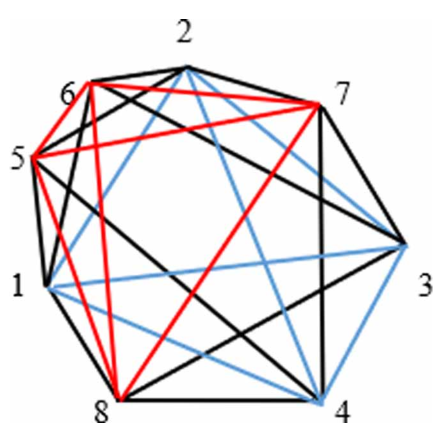


Figure 3. The 4 – cross - polytope



If we designate the newly formed vertices by a pair of vertices of the corresponding edges of the original tetrahedron 1234, then these are the next vertices (1,2), (1, 3), (1, 4), (2, 3), (2, 4), (3, 4). Among these newly formed vertices, opposite vertices can be distinguished, given the opposite edges of the original 1234 tetrahedron. These opposite vertices also form pairs:

$(2,3)$ (1,2) (1,3)
(1,4) (4,3) (2,4)

If one connected the remaining vertices of edges, leaving pairs:

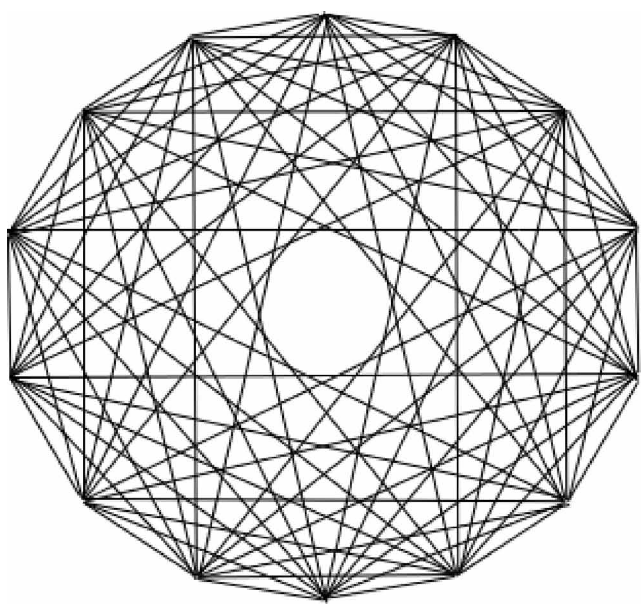
1 2 3 4
7 8 5 6

unconnected, so can to get a 7 – cross - polytope. In a topologically equivalent form, this polytope of dimension 7 is shown in Figure 4.

From the general expression for the number of elements of the dimension and in the *d* - cross - polytope (Zhizhin, 2013, 2014c, 2018) $f_i(d) = 2^{1+i} C_d^{d-1-i}$ it follows that the number of vertices in this polytope $f_0 = 2 \cdot C_7^6 = 14$, the number of edges $f_1 = 2^2 \cdot C_7^5 = 84$, the number of triangle faces $f_2 = 8 \cdot C_7^4 = 280$, the number of tetrahedrons $f_3 = 16 \cdot C_7^3 = 560$, the number of four – dimension simplexes $f_4 = 32 \cdot C_7^2 = 672$, the number of five – dimension simplexes $f_5 = 64 \cdot C_7^1 = 448$, the number of six – dimension simplexes $f_6 = 128$.

If one connected a pair of tetrahedrons to the edges of the tetrahedron 5678, so can to obtain six more vertices (5, 6), (5.7), (5, 8), (6, 7), (6, 8), (7, 8). Opposite ones can be distinguished among these vertices, considering the opposite of the edges of the tetrahedron 5678:

Figure 4. The 7 – cross - polytope



(5,6) (5,8) (6,8)
(8,7) (6,7) (5,7)

If one connected the remaining vertices with edges, leaving pairs:

1 2 3 4 (2,3) (1,2) (1,3) (5,6) (5,8) (6,8)
7 8 5 6 (1,4) (4,3) (2,4) (8,7) (6,7) (5,7)

unconnected, so can to get a 10 – cross - polytope. In this polytope the number of vertices is $f_0(10) = 2 \cdot C_{10}^{9} = 20,$ the number of edges is $f_1(10) = 2^2 \cdot C_{10}^{8} = 180,$ the number of triangle faces $f_2(10) = 8 \cdot C_{10}^{7} = 960,$ the number of tetrahedrons $f_3(10) = 16 \cdot C_{10}^{6} = 3360,$ the number of four – dimension simplexes $f_4(10) = 32 \cdot C_{10}^{5} = 8064,$ the number of five – dimension simplexes $f_5(10) = 64 \cdot C_{10}^{4} = 13440,$ the number of six – dimension simplexes $f_6(10) = 128C_{10}^{3} = 15360,$ the number of seven – dimension simplexes $f_7(10) = 256C_{10}^{2} = 11520,$ the number of eight – dimension simplexes $f_8(10) = 512C_{10}^{1} = 5120,$ the number of nine – dimension simplexes $f_9(10) = 1024.$

Continuing to attach tetrahedrons to a cluster of 20 vertices, keeping the order of attachment, as in the previous steps, a cluster of 26 atoms can be obtained. This will be the 13 - cross – polytope. In this polytope, the number of vertices is $f_0(13) = 2 \cdot C_{13}^{12} = 26$ and the number of tetrahedrons is $f_3(13) = 2^4 \cdot C_{13}^{9} = 45760$. Thus, instead of a cluster in the form of four interpenetrating icosahedrons in three - dimensional space, the image of this cluster in the space of dimension 13 in the form of a convex standard cross - polytope can serve. Two such clusters make up an elementary cell of γ - brass. Thus, it was proved that the addition of tetrahedrons to a γ - brass cluster of 8 atoms, having the form of a 4 – cross - polytope, leads to the creation of a number of shells, and the dimension of the cluster when each shell is attached increases by three. The number of elements of different dimensions in a cluster for any shell number *n* (*n* = 0, 1, 2, ...) is determined by the formula established earlier for *d* - cross - polytopes. Q.E.D.

Clusters of Bergman, Samson and R – Phases

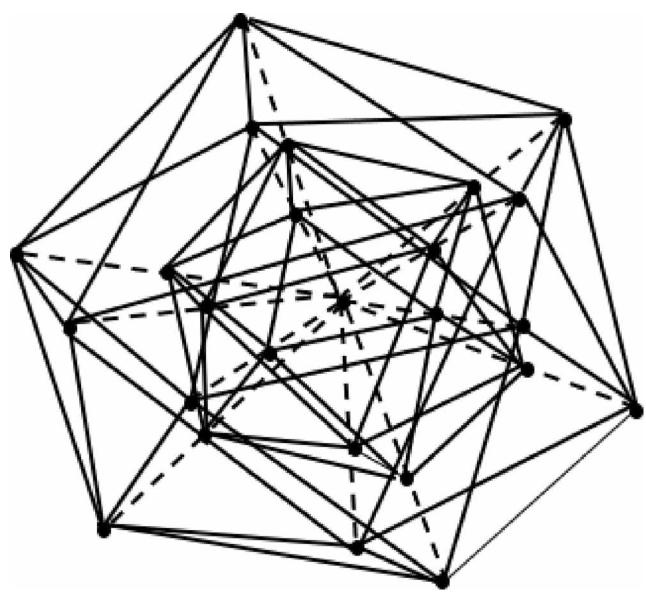
In many metal alloys (for example, Al_5CuLi_3, Mg_6Pd, Mg_{32} (Al, Zn)$_{49}$ and etc.) there are clusters in which the initial element is an icosahedron with a central atom (in contrast to Mackay's clusters). The extension of the tetrahedrons to the outer surface of the icosahedron leads to the formation of the next convex shell. This process can be continued and a series of larger convex hulls can be obtained. The location of the vertices on each convex hull is often determined by the author, based on the author's commitment to some of the ideas prevailing at a given time. So, there were clusters, designated by the name of the authors (cluster of Bergman, cluster of Samson, three - contahedron of Pauling). However, to determine the dimension of these clusters with a central atom, it is important that an icosahedral surface can be distinguished on all these outer shells. The sizes of triangles on these surfaces naturally increase as one moves to more and more distant shells. Such clusters will be called icosahedral complexes with a central atom.

Theorem 3: The dimension *d* of icosahedral complexes with a central atom equal *n* + 3, where *n* is the number of the shells in the complexes.

Proof: The icosahedral with a central atom has 13 vertices $\left(f_0 = 13\right)$, 42 edges $\left(f_1 = 42\right)$, 50 flat triangle faces $\left(f_2 = 50\right)$, 21 three – dimensional faces (20 triangle pyramids and 1 icosahedron) $\left(f_3 = 21\right)$. Substituting these values into Equation (1) one have 13 – 42 + 50 – 21 = 0. This proves that the icosahedron with its center has a dimension of 4. If one continue the edges going from the center of the icosahedron (Figure 5), and on these edges at the appropriate distance arrange more atoms forming the second icosahedron of a larger size, such a construction of two icosahedra with a common center will have 25 vertices $\left(f_0 = 25\right)$, 84 edges $\left(f_1 = 2 \cdot 30 + 2 \cdot 12 = 84\right)$, 100 flat faces $\left(f_2 = 2 \cdot 20 + 2 \cdot 30 = 100\right)$, 42 three - dimensional faces $\left(f_3 = 2 \cdot 20 + 2 = 42\right)$, 3 four - dimensional faces $\left(f_4 = C_3^2 = 3\right)$. Substituting these values in the Equation (1) we have 25 - 84 + 100 – 42 + 3 = 2. This proves that the two icosahedrons with common center have a dimension 5.

Note that the number of four - dimensional faces in this case includes a smaller icosahedron with a center, a larger icosahedron with a center, and the space between two icosahedrons. Indeed, for this space one have 24 vertices $\left(f_0 = 24\right)$, 72 edges $\left(f_1 = 2 \cdot 30 + 12 = 72\right)$, 70 flat faces $\left(f_2 = 2 \cdot 20 + 30 = 70\right)$, 22 three - dimensional faces $\left(f_3 = 20 + 2 = 22\right)$. Substituting these values into the Equation (1) one have 24 - 72 + 70 – 22 = 0. This proves that the space between two icosahedrons has a dimension 4. The total number of four - dimensional elements in this case is determined by the number of combinations between the three characteristic elements of the construction (the center and two icosahedral surfaces) of two elements. Any of these combinations gives a four - dimensional element. If one continue again the edges coming from the center of the icosahedrons, and on these edges one construct the third icosahedron of a still larger size, then such a construction will have 37 vertices $\left(f_0 = 25 + 12 = 37\right)$, 126 edges $\left(f_1 = 3 \cdot 30 + 3 \cdot 12 = 126\right)$, 150 flat faces $\left(f_2 = 3 \cdot 20 + 3 \cdot 30 = 150\right)$, 63 three - dimensional faces $\left(f_3 = 3 \cdot 20 + 3 = 63\right)$, 6 four - dimensional faces $\left(f_4 = C_4^2 = 6\right)$, 4 five – dimensional faces $\left(f_5 = C_4^3 = 4\right)$. Substituting these values in the Equation (1) we have 37 - 126 + 150 – 63 + 6 - 4 = 0. This proves that the three icosahedrons with common center have a dimension 6.

Figure 5. Two icosahedrons with a common center



The total number of four - dimensional elements in this case is determined by the number of combinations between the four characteristic elements of the construction (the center and three icosahedral surfaces) of two elements. Any of these combinations gives a four - dimensional element. The total number of five - dimensional elements in this case is determined by the number of combinations between the three characteristic elements of the construction (the center and three icosahedral surfaces) of three elements. Any of these combinations gives a five - dimensional element. These constructions can be continued. However, it is now possible to write general expressions for the numbers of elements of different dimensions in a cluster with a center for arbitrary number *n* of shells of icosahedra and to give a formula for calculating its dimension. So, in the *n* - shell cluster of icosahedrons with a center, we have:

$$f_0 = n \cdot 12 + 1, f_1 = n \cdot 30 + n \cdot 12, f_2 = n \cdot 20 + n \cdot 30, f_3 = n \cdot 20 + n,$$
$$f_4 = C_{n+1}^2, f_5 = C_{n+1}^3, \ldots, f_{n+2} = C_{n+1}^n. \quad (5)$$

Substituting these values in the Equation (1) you can see that in this case the left side of the Euler-Poincaré Equation (1) takes the form:

$$\sum_{i=0}^{d-1} (-1)^i f_i(P) = 1 - n + \sum_{k=2}^{n} C_{n+1}^k (-1)^k \quad (6)$$

To calculate the sum on the right side of Equation (6), we use the expression (4) for the alternating series of combinations (Vilenkin, 1969). From the series (4), taking into account the equalities $C_n^0 = C_n^n = 1, C_n^1 = n$, it follows that when n is even the sum $\sum_{k=2}^{n-1} C_n^k (-1)^k$ in the right side of Equation (3) is $n - 2$ while n is odd the sum is equal to n. Therefore, the right side of Equation (6) coincides with the right side of Equation (1). This proves that the figures in question are closed convex polytopes and they satisfy the Euler-Poincaré equation. At the same time, from Equation (5), since $f_{n+3} = C_{n+1}^{n+1} = 1$, it follows that the dimension of a cluster of *n* - icosahedrons with an atom in a common center is equal $d = n + 3$. Q.E.D.

Thus, as in the Mackay clusters, the dimension of clusters of several icosahedra with one common central atom increases linearly with the number of shells. The dimension of these clusters is greater than the dimension of the corresponding Mackay clusters by one due to the presence of an atom in a common center. The outer surface of the clusters of Bergman, Samson, and R - phases (Lord et al., 2006) outwardly seems to be different from the icosahedron. However, this difference is not significant. For example, in the Bergman cluster of 45 atoms, the outer surface is supposed to consist of rhombuses. Can to note by construction that it is not, it is the icosahedron. For example, the clusters from Mg_{32} (Al, Zn) $_{49}$ was specifically decided to deform in order to bring it closer to Pauling's three - contahedron (Bergman et al., 1952, 1957). In the Samson cluster of 105 atoms of alloy Mg_6Pd (Samson, 1972), the outer surface is a truncated icosahedron. It is easy to get an icosahedron from this surface, connecting the centers of the pentagons, especially since the initial construction is based on tetrahedrons. The surfaces of the R - phase clusters from Mg_{32} (Al, Zn)$_{49}$, Mo – Cu – Cr, Al_5CuLi_3 also consist of elements of icosahedral surfaces (Bergman et al., 1952, 1957; Komura et al., 1960; Audier et al., 1998). Therefore, the dimensions of these clusters can be calculated from the formulas obtained in this work, taking into account the number of shells in these clusters. Since the Bergman cluster has two icosahedral shells, according to Theorem 3 its dimension is 5. Since the Samson cluster has three shells, its dimension is 6. Since the R - phase cluster has four shells, its dimension is 7.

The Dimension of Metallic Clusters of Several Shells in the Form of Plato's Bodies

The icosahedron is only one of Plato's bodies found in the skeleton of metal clusters (Gubin, 2019). Suppose there is a cluster, each shell of which is a convex regular three - dimensional polyhedron (Plato's body) with some possible number of vertices *n* and the same for all shells of this cluster. The flat sides of the shells are a regular *m* - corner. All shells of this cluster differ only in size and have a common center. Assume that the number of flat edges in the shell is *j*. We denote a shell satisfying the indicated conditions S_j. Then the following statement is true.

Theorem 4: The dimension *d* of a cluster of *N* shells with a common center is $N + 2$, if there is no atom in the common center, and is equal to $N + 3$, if there is an atom in the common center.

Proof: Denote by the symbol *t* the number of edges emanating from each vertex of the shell S_j. Then the total number of edges of the shell is $nt / 2$, and the number of faces of the shell is $j = nt / m$. The number *j* in Plato's body also gives the form of the shell, i.e. sets the numbers *n, m, t* (Table 1).

Let a shell with the number of faces *j* and be given. Therefore, the number of vertices n_j, the number of sides m_j at the flat face, the number of edges t_j emanating from each vertex are given. Consider two shells of different sizes with a common center, arranged so that every two corresponding vertices of both shells are on the same straight line connecting them with a common center (there is no atom in the center). Then the space between the shells is filled with prisms, the bases of which are flat faces of the larger and smaller shells. The number of these prisms is equal to the number of faces of the shell, i.e. *j*. The number of vertices in a polytope of two shells is $2n_j = f_0$. The number of edges of this polytope, taking into account the edges connecting the corresponding vertices of the shells, is $n_j t_j + n_j = f_1$. The number of flat edges in a polytope is equal to twice the number of flat edges in each shell and the number of edges in one of the shells, i.e.:

$$2j + \frac{n_j t_j}{2} = f_2$$

The number of three - dimensional figures in the polytope is equal to $j + 2 = f_3$. Substitute these numbers in the Equation (1) Euler – Poincare:

$$2n_j - n_j(t_j + 1) + 2j + \frac{n_j t_j}{2} - j - 2 = (n_j - \frac{n_j t_j}{2} + j) - 2 = 0$$

Table 1. The relationship between the geometric characteristics in the bodies of Plato

J	*n*	*m*	*t*	**Polyhedron**
4	4	3	3	Tetrahedron
6	8	4	3	Cube
8	6	3	4	Octahedron
12	20	5	3	Dodecahedron
20	12	3	5	Icosahedron

There $\left(n_j - \frac{n_j t_j}{2} + j\right) = 2$ on the Equation (1) for the polytope of dimension 3.

This proves that a polytope composed of two shells S_j with a common center (in the absence of an atom in the center) has dimension 4 for any possible *j*. If the cluster consists of three shells S_j with a common center, then $f_0 = 3n_j$. The number of edges in this cluster, taking into account the edges connecting of the corresponding vertices in shells S_j, is equal to $f_1 = 3\frac{n_j t_j}{2} + 2n_j$. The number of two - dimensional faces is $3j + n_j t_j = f_2$. The number of three - dimensional faces is $2j + 3 = f_3$. The number of four – dimensional faces is $f_4 = C_3^2 = 3$. Substitute these numbers in the Equation (1) Euler – Poincare:

$$3n_j - n_j\left(\frac{3}{2}t_j + 2\right) + 3j + n_j t_j - (2\,\mathrm{j}+3) + 3 = n_j - \frac{n_j t_j}{2} + j = 2$$

This proves that dimension of the cluster of three shells S_j is equal to 5. Can to write general expressions for the numbers of elements of different dimensions in a cluster with an arbitrary number *N* of shells S_j and to give a formula for calculating its dimension. So, in the *N* - shell cluster of shells S_j, we have:

$$f_0 = Nn_j, f_1 = N\frac{n_j t_j}{2} + (N-1)n_j, f_2 = Nj + (N-1)\frac{n_j t_j}{2}, f_3 = (N-1)\,\mathrm{j}+ N,$$
$$f_4 = C_N^2, f_5 = C_N^3, \ldots, f_{N+1} = C_N^{N-1} \tag{7}$$

Substituting the values (5) in the Equation (1) and opening the brackets you can see that in this case the left side of the Euler-Poincaré Equation (1) takes the form:

$$\sum_{i=0}^{d-1}(-1)^i f_i(P) = 2 - N + \sum_{k=2}^{N-1} C_N^k (-1)^k \tag{8}$$

To calculate the sum on the right side of Equation (8), we use the expression for the alternating series of combinations (Vilenkin, 1969):

$$C_N^0 - C_N^1 + C_N^2 - \ldots + (-1)^N C_N^N = 0 \tag{9}$$

From the series (7), taking into account the equalities $C_N^0 = C_N^N = 1, C_N^1 = N$, it follows that when *N* is even the sum $\sum_{k=2}^{N-1} C_N^k (-1)^k$ in the right side of Equation (8) is *N* - 2 while *N* odd the sum is equal to *N*. Therefore, the right side of Equation (8) coincides with the right side of Equation (1). This proves that the figures in question are closed convex polytopes and they satisfy the Euler – Poincaré equation.

At the same time, from Equation (7), since $f_{N+2} = C_N^N = 1$, it follows that the dimension of a cluster of *N* shells S_j with a common center if at center not atoms is equal *d* = *N* + 2.

One now considers a cluster of several shells S_j with a common center in which the atom is located. The shell S_j with a central atom has $n_j + 1 = f_0$ vertices, $\frac{n_j t_j}{2} + n_j = f_1$ edges, $\frac{n_j t_j}{2} + j = f_2$ flat faces, $j + 1 = f_3$ three – dimensional faces. Substituting these values in the Equation (1) we have:

$$n_j + 1 - \left(n_j + \frac{n_j t_j}{2}\right) + j + \frac{n_j t_j}{2} - \left(j - 1\right) = 0$$

This proves that the shell S_j with its center has a dimension of 4. If one continue the edges going from the center of the shell S_j to its vertices and at the appropriate distance arrange more atoms forming the second a shell S_j of a larger size. Such a construction of two the shells S_j with a common atom in center will have $2n_j + 1 = f_0$ vertices, $n_j t_j + 2n_j = f_1$ edges, $2j + n_j t_j = f_2$ flat faces, $2j + 2 = f_3$ three - dimensional faces, $f_4 = C_3^2 = 3$ four - dimensional faces. Substituting these values in the Equation (1) you can get:

$$2n_j + 1 - 2n_j(1 + t_j / 2) + 2j + n_j t_j - (2j + 2) + 3 = 2$$

This proves that the two shells S_j with common atoms in the center has a dimension 5.

If one continue again the edges coming from the center of the shells S_j, and on these edges one construct the third shell S_j of a still larger size, then such a construction will have $f_0 = 3n_j + 1$ vertices, $f_1 = 3\frac{n_j t_j}{2} + 3n_j$ edges, $f_2 = 3j + 3\frac{n_j t_j}{2}$ flat faces, $f_3 = 3j + 3$ three - dimensional faces, $f_4 = C_4^2 = 6$ four - dimensional faces, $f_5 = C_4^3 = 4$ five – dimensional faces. Substituting these values in the Equation (1) you can get:

$$3n_j + 1 - 3\left(n_j + \frac{n_j t_j}{2}\right) + 3\left(j + \frac{n_j t_j}{2}\right) + 3\left(j + 1\right) + 6 - 4 = 0$$

This proves that cluster of the tree shells S_j with common atom at center has a dimension 6.

Can to write general expressions for the numbers of elements of different dimensions in a cluster with a center for arbitrary number *N* of shells S_j and to give a formula for calculating its dimension. So, in the cluster of *N* shell S_j with atom in a common center, we have:

$$f_0 = Nn_j + 1, f_1 = N\frac{n_j t_j}{2} + Nn_j, f_2 = Nj + N\frac{n_j t_j}{2}, f_3 = Nj + N,$$
$$f_4 = C_{N+1}^2, f_5 = C_{N+1}^3, \ldots, f_{N+2} = C_{N+1}^N \quad (10)$$

Substituting these values in the Equation (1) you can see that in this case the left side of the Euler-Poincaré Equation (1) takes the form:

$$\sum_{i=0}^{d-1}(-1)^i f_i(P) = 1 - N + \sum_{k=2}^{N} C_{N+1}^{k}(-1)^k \quad (11)$$

To calculate the sum on the right side of Equation (8), we use the expression (7). From the series (7), taking into account the equalities $C_N^0 = C_N^N = 1, C_N^1 = N$, it follows that the sum $\sum_{k=2}^{N} C_{N+1}^{k}(-1)^k$ in the right side of Equation (11) is $N + 1$ for N even and N -1 for N odd. Therefore, the right side of Equation (11) coincides with the right side of Equation (1). This proves that the figures in question are closed convex polytopes and they satisfy the Euler-Poincaré equation.

At the same time, from Equation (10), since $f_{N+3} = C_{N+1}^{N+1} = 1$, it follows that the dimension of a cluster of N shells S_j with an atom in a common center is equal $d = N + 3$. Q.E.D.

Clusters of the Hyper-Rhombohedrons

When analyzing the diffraction pattern of intermetallic compounds of Al_6Mn (Shechtman, et al.,1984), $Ti_{54}Zr_{26}Ni_{20}$ (Zang, & Kelton, 1993), $Al_{70}Fe_{20}W_{10}$ (Mukhopadhyay, et al., 1993), $Al_{72}Ni_{20}Co_8$ (Eiji, Yanfa, & Pennycook, 2004) it was found (Zhizhin, 2014, 2017, 2018), that the unit cell of the structure created by the luminous points of the diffraction patterns is a figure of dimension 4, called the golden hyper - rhombohedron. It consists of eight rhombohedrons, with angles in the flat edges defined by the golden section. It contains 16 vertices (Figure 6).

This figure provides the translational symmetry of quasicrystals in the space of higher dimension. The golden hyper - rhombohedron can be considered a cluster of intermetallic compounds, since the luminous points in the diffraction patterns are lattice nodes, which reflect the rays passing through the metal alloy. The products of the golden hyper - rhombohedron on other geometric figures lead to the formation of clusters of higher dimensions. Definitions and research works of various geometric shapes are given in the monographs of the author (Zhizhin, 2017, 2018). In Figure 7 and Figure 8, as an example, the products of the golden hyper - rhombohedron on a triangle and a tetrahedron are shown, correspondingly.

Figure 6. The golden hyper-rhombohedron

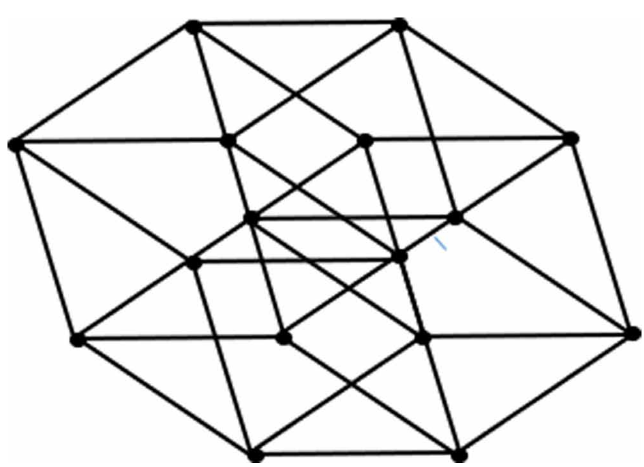


Figure 7. The product of golden hyper - rhombohedron on a triangle

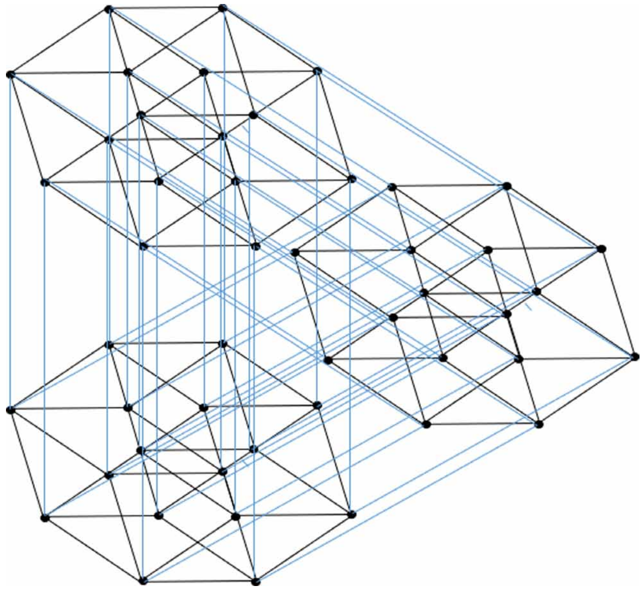
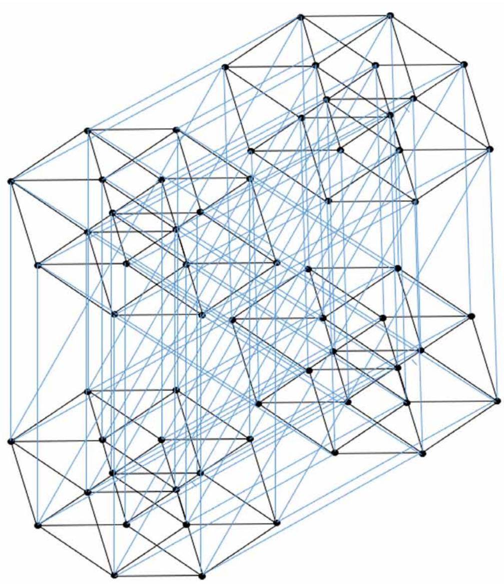


Figure 8. The product of golden hyper - rhombohedron on a tetrahedron



Since the dimension of the product of the figures is equal to the sum of the dimensions of the factors, the dimension of the product of the golden hyper - rhombohedron by a triangle is 6, and the dimension of the product of the golden hyper - rhombohedron by the tetrahedron is 7. The number of vertices in the product of the figures is equal to the product of the numbers of the vertices of the factors. Therefore, the number of vertices in the product of the golden hyper - rhombohedron on a triangle is equal to 48, and the number of vertices in the product of the golden hyper - rhombohedron on a tetrahedron is 64.

CONCLUSION

For the first time, analytical expressions are obtained for calculating the dimension of multi - shell clusters depending on the number of shells. These expressions are applicable to clusters consisting of shells in the form of an icosahedron with a common center, if an atom is located or dislocated in this center. From the obtained analytical formulas in it follows that in both cases the dimension of the clusters increases linearly with an increase in the number of shells. Thus, for the clusters of Mackay (Mackay, 1962), Bergman (Bergman et al., 1952, 1957), Samson (Samson, 1972) known in the literature, which can be approximately described by such multi - shell models, expressions are obtained for calculating their dimensions and proved that they have a higher dimension. It should be noted an interesting fact that the clusters of γ - brass studied for a long time turned out to have geometry of a high - dimensional cross-polytope. Consequently, not only extended alloys of intermetallic compounds have a higher dimension, but also isolated compounds of intermetallic compounds in the form of clusters have a higher dimension. Clusters, connecting with each other, lead to the formation of new clusters with an even higher dimension. This also applies to the hyper - rhombohedron, as a cluster of quasicrystals. This is demonstrated in this paper. In the case of complex clusters of intermetallic compounds containing a large number of atoms and formations in various geometric forms, it is difficult to determine their dimension. However, it is safe to say on the basis the conducted research, that they have a higher dimension.

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KEY TERMS AND DEFINITIONS

Diffraction: A wide range of phenomena occurring in the propagation of waves in heterogeneous environments in the space.

Dimension of the space: The member of independent parameters needed to describe the change in position of an object in space.

Fractal: The set is self-similar, i.e. uniformity at different scales.

Golden Gyper-rhombohedron: Polytope in 4-dimensional space with facets as rhombohedron and metric characteristics associated the golden section.

Polytope: Polyhedron in the space of higher dimension.

Quasicrystal: A solid body, characterized by symmetry without translation in 3-dimensional Euclidean space.