Topological Characterization of Cellular Structures

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Abstract: In order to characterize quantitatively the local topological structure of cellular systems a new method has been developed. First, we analyzed the topological properties of infinite periodic cellular structures, and then the general theoretical results obtained have been adapted to the local topological characterization of 2-dimensional finite cellular surface systems. The concept of this new approach is based on the use of the so-called double toroidal embedding (DT embedding) by which a finite cellular system defined on a torus can be generated from an infinite periodic cellular system. The DT embedding is a special mapping, which enables to preserve all the local topological properties of the original infinite periodic cellular system. As a result of performing a DT embedding, so-called neighborhood coefficients can be generated. The neighborhood coefficients are scalar topological invariants, by which the local topological structure of cellular systems can be quantitatively evaluated and compared. Moreover, by investigating the relationship between the neighborhood coefficients and other local topological quantities, we verify that the validity of the Weaire-Fortes identity can be extended to a broad class of infinite periodic cellular systems and 2-d finite cellular surface systems (i.e. generalized fullerene-like surface structures). Finally, it has been shown that the traditional definition of fullerenes can be generalized by introducing the notion of the cellular fullerene, which is considered as a finite cellular system defined on a 2-d unbounded, closed and orientable surface.

Keywords: cell, embedding, toroidal graphs, Weaire-Fortes identity, corona, fullerene

1. Introduction

In various fields of material sciences, many interesting 2- and 3-dimensional structures (fullerenes, nanotubes, froths, metal foams, polycrystals) can be

modeled by a special arrangement of space filling polygons and polyhedra (i.e. 2- or 3- dimensional polytopes) and thus can be considered as finite or infinite cellular systems. Over the past two decades, most studies have concentrated on 2-d cellular structures which may be represented by infinite, planar networks, usually with trivalent vertices (i.e. three edges at each vertex) [1-6]. This paper presents a general method, which is designated primarily to the topological evaluation of infinite periodic and finite cellular systems composed of d-dimensional polyhedra (polytopes) where $d \geq 2$.

The proposed method is based on the application of a double toroidal embedding (DT embedding) by which a finite space-filling cellular system defined on a torus can be generated. The DT embedding is considered as a one-to-one mapping of the topological types, which enables to preserve all the local topological properties of the original infinite periodic cellular system. It will be shown that, after performing a DT embedding, so-called neighborhood coefficients can be computed, by which the local topological structure of periodic cellular systems can be simply analyzed and compared. Additionally it will be verified that the validity of the Weaire-Fortes identity [2-4] playing a key role in the topological description of 2-dimensional random cellular patterns, could be extended to finite dimensional periodic cellular systems. The fundamental results concerning the extension of the Weaire-Fortes identity are represented by Eqs. (33 and 34). Finally, it is shown that the traditional definition of fullerenes can be generalized by introducing the notion of the cellular fullerene, which is considered as a finite cellular system defined on a 2-d unbounded, closed and orientable surface.

2. Locally finite periodic cellular systems

The most important type of infinite d-dimensional cellular systems is the so-called countable cellular system [7]. A countable cellular system is considered as a face-to-face tiling (tessellation) of d-dimensional Euclidean space denoted by $\boldsymbol{E}^{(d)}$ by a countable set of d-dimensional compact combinatorial polyhedra (polytopes). Each d-dimensional polyhedron called a cell is topologically equivalent (homeomorfic) to a d-dimensional sphere. A countable cellular system denoted by $\boldsymbol{\Omega}_{\mathbf{d}}$ is defined by taking into consideration the fulfillment of the following requirements:

i. $\boldsymbol{\Omega}_{\mathbf{d}}$ can be represented as

$$\boldsymbol{\Omega}_{\mathbf{d}} = \left\{ A_j \,\middle|\, j \in I_P \ldots \text{and} \ldots \bigcup_j A_j = \mathbf{E}^{(\mathbf{d})} \right\} \tag{1}$$

where I_P is the index set of positive integers, A_j is the jth cell (polyhedron) in $\boldsymbol{\Omega}_{\mathbf{d}}$.

ii. The k-dimensional faces of polyhedra included in $\boldsymbol{\Omega_d}$ (k=0,1,2,…,d-1) are also compact combinatorial polyhedra, and the maximum number of k-dimensional faces is less then γ_k, where γ_k are finite positive integers for k=0,1,2,…d-1. (The 0-dimensional and 1-dimensional faces of polyhedra are called vertices and edges, respectively.)

iii. Polyhedra can be included in a d-dimensional sphere with a finite radius, which guaranties that the "size" of cells is finite [7].

iv. All of the k-dimensional faces of a d-dimensional polyhedron have a positive k-dimensional volume (measure) for k=1,2,…d.

v. Each (d-1) -dimensional face between cells is the common face of two different cells (polyhedra) exactly.

vi. Additionally it is assumed that $\boldsymbol{\Omega_d}$ is locally finite [7]. By definition, a countable cellular system is called locally finite if there exists a positive number ρ for any arbitrary point P_x in $\boldsymbol{E^{(d)}}$, such that every d-dimensional sphere $G(P_x,\rho)$ with radius ρ and center point P_x, contains finite number cells from $\boldsymbol{\Omega_d}$ only. This definition implies that there are no singularity points of cells in the cellular system. For each vertex X (0-dimensional face) in $\boldsymbol{\Omega_d}$ the number of edges (1-dimensional faces) incident to X is called the valency of X, denoted by r (or r(X)). If all of the vertices of have the same valency R, then $\boldsymbol{\Omega_d}$ is said to be a regular, or R-valent cellular system.

For purposes of our investigations the most important groups of locally finite cellular systems are the periodic cellular systems. A locally finite cellular system $\boldsymbol{\Omega_d}$ is called periodic, if there exists a d-dimensional parallelepiped $\boldsymbol{\Pi_d}$ represented by a linearly independent vector system ($\mathbf{v_1}$, $\mathbf{v_2}$,… $\mathbf{v_k}$, ...$\mathbf{v_d}$) for which relationships

$$\boldsymbol{\Pi_d} \subset \left\{ \bigcup A_j \middle| A_j \in \boldsymbol{\Omega_d} \right\} \tag{2a}$$

and

$$\mathbf{E^{(d)}} = \left\{ \bigcup \mathbf{B_v} \middle| \mathbf{B_v} = \boldsymbol{\Pi_d} + \sum_{k=1}^{d} \varepsilon_k \mathbf{v_k}, ...\varepsilon_k \in I_\varepsilon \right\} \tag{2b}$$

are fulfilled, where ε_k are integers for k = 1,2,….d, and I_ε is the set of integers [7].

In the following, it is supposed that $\boldsymbol{\Omega_d}$ is a locally finite periodic cellular system (LFPC system). From the previous considerations it follows, that parallelepiped $\boldsymbol{\Pi_d}$ can be covered by the union of a finite set of cells belonging to $\boldsymbol{\Omega_d}$. This implies that a LFPC system is generated from a finite set of polyhedra of combinatorially different types.

It will be shown that the topological description of a locally finite periodic cellular system (LFPC system) can be traced back to the topological characterization of an appropriately constructed finite cellular system. Parallelepiped $\mathbf{\Pi_d}$ has been chosen in such a way, that it has a minimum volume. It should be emphasized that this parallelepiped $\mathbf{\Pi_d}$ is not uniquely defined. They can be constructed in different manners; however, their common property is that their d-dimensional volumes are identical.

There is no loss in generality in assuming the following: By using an appropriately selected homogenous linear transformation, parallelepiped $\mathbf{\Pi_d}$ can be mapped into a d-dimensional unit cube. This unit cube $\mathbf{\Pi_{d,U}}$ which is called "a unit domain" in the classical crystallography is given by

$$\mathbf{\Pi_{d,U}} = \{\mathbf{x} = (x_1, x_2,\ldots x_k,\ldots x_d) \mid 0 \le x_k \le 1 \text{ and } k = 1,2,\ldots d\} \qquad (3)$$

This simple transformation makes it possible to replace the original LFPC system by a "standardized" periodic cellular system generated by translations of $\mathbf{\Pi_{d,U}}$. The only difference is that the standardized LFPC system is composed of unit cubes instead of parallelepipeds. Since a linear transformation represents a "topology preserving" onto-to-one mapping, this implies that the original and the transformed periodic cellular systems are topologically equivalent. In the further investigations, it will be supposed that the LFPC system $\boldsymbol{\Omega_d}$ is a standardized cellular system.

3. Finite cellular systems constructed by using a double toroidal embedding

From a LFPC system, finite cellular systems of a toroidal type can be constructed in several ways. In the following, it will be demonstrated that starting with a d-dimensional LFPC system and by using the so-called double toroidal embedding, it is always possible to construct a uniquely defined finite cellular system represented by a torus in the (d+1) dimensional Euclidean space, which is advantageously applicable to the local topological evaluation of infinite periodic cellular systems.

In order to generate a finite cellular system from a standardized LFPC system, consider a unit domain $\mathbf{\Pi_{d,U}}$ defined by Eq. (3). As a first step, let us construct a so-called identification region $\mathbf{S_d}$, which is composed of 2^d unit domains, as follows

$$\mathbf{S_d} = \{\mathbf{x} = (x_1, x_2,\ldots x_k,\ldots x_d) \mid 0 \le x_k \le 2 \text{ and } k = 1,2,\ldots d\} \qquad (4)$$

As can be stated, $\mathbf{S_d}$ is also a d-dimensional cube with edge length of 2. As a second step, let us construct a finite toroidal cellular system $\boldsymbol{R_d}$ (FTC system) by

gluing (identifying) the opposing k-dimensional face pairs (edges, vertices, etc.) of $\mathbf{S_d}$ (k=0,1,2,….d-1).

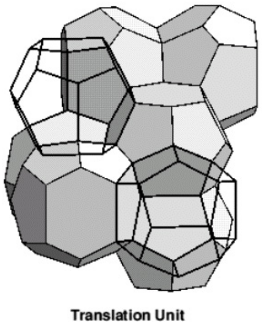

Fig.1 The 3-dimensional, periodic Weaire-Phelan cellular system

This mapping is called the double toroidal embedding (DT embedding) of the d-dimensional LFPC system, because $\boldsymbol{R_d}$ represents a torus in the (d+1)-dimensional Euclidean space. As an example, **Fig. 1** shows a two-component, space-filling periodic polyhedral system. In this 3-dimensional LFPC system that was discovered by Weaire and Phelan, the space-filling unit domain consists of six tetrakaidecahedra (14-sided Goldberg polyhedra) and two irregular pentagonal dodecahedra (12-sided polyhedra) [8].

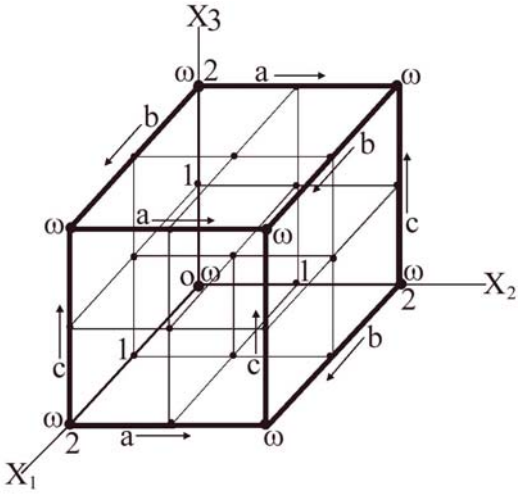

Fig.2 Identification region $\mathbf{S_3}$ generated by 8 unit domains to the DT embedding of a 3-d LFPC system

In **Fig. 2**, the construction of the identification region of a 3-dimensional LFPC system is illustrated. As can be seen, this is the union of 8 unit domains. The

arrows a, b and c are used to specify a direction for the edges, and this direction must be respected when gluing is done. The eight vertex points of the identification region $\mathbf{S_3}$ are joined to form a single point ω of the resulting toroidal system.

Fig. 3 demonstrates the general concept of the DT embedding of a 2-dimensional LFPC system. As an example, in **Fig. 4**., the DT embedding is shown for a 2-d periodic cellular system, which includes 4- and 8-sided polygons. The resulting FTC system is also composed of four 4-sided and four 8-sided cells (See Fig 4.c). The number of cells is 8, the number of edges is 24, and the number of vertices is 16. As it is expected, the Euler-characteristic of this finite system defined on the torus surface is zero.

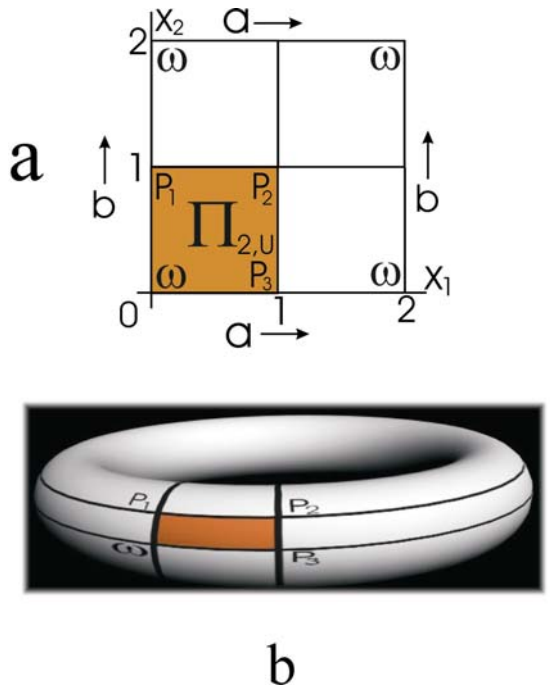

Fig.3 Principle of the DT embedding of a 2-d LFPC system (a) The 2-d identification region $\mathbf{S_2}$ composed of 4 unit domains, (b) The corresponding FTC system defined on a torus

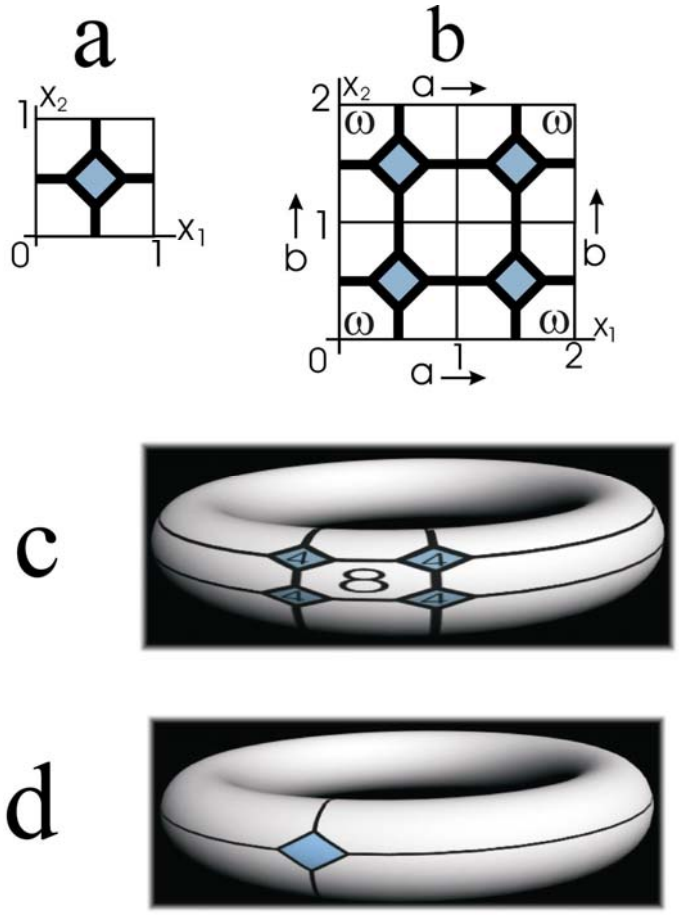

Fig.4 Example of the toroidal embedding of a 2-d LFPC system (a) The unit domain $\mathbf{\Pi_{2,U}}$, (b) The corresponding identification region $\mathbf{S_2}$, (c) The DT embedding performed on the torus, (d) The traditional toroidal embedding of the 2-d LFPC system by using a single unit domain only

The basic properties of the DT embedding and of FTC systems are as follows:

a. The total number of cells in $\mathbf{S_d}$ is equal to $N_{d,U} \times 2^d$, where $N_{d,U}$ denotes the number of cells in the unit domain.

b. The resulting FTC system preserves all the topological properties of the original LFPC system. This is due to the following fact: In cellular systems generated by a DT embedding, each (d-1)-dimensional face is shared by two different neighbor cells exactly. Since a DT embedding is a topology preserving one-to-one mapping between the LFPC and FTC

system this implies that an LFPC system can be unambiguously reconstructed from the corresponding FTC system generated by a DT embedding. It should be noted, that using a single unit domain could also perform a toroidal embedding. Unfortunately, in certain cases, if we use only one unit domain to generate a finite toroidal cellular system, as a result of this procedure the local topological properties characterizing the neighborhood structure of cells can change radically. Consequently, the classical toroidal embedding cannot be applicable to every case. As an example, this is illustrated in Fig 4.d. Due to the toroidal embedding with a single unit domain, the original topological structure of the 2-dimensional LFPC system depicted in Fig. 4.a, has been degenerated. In this case, the number of cells is 2, the number of edges is 6, and the number of vertices is 4, the Euler-characteristic is zero. As it can be stated Fig 4.d shows the conventional 2-cell embedding of the complete graph K_4 in the torus, where one of the two cells is 4-sided, while the other is 6-sided. This is explained by the fact that in this toroidal cellular system there exist two edges, which belong to the same 6-sided cell. This implies that the original LFPC system shown in Fig. 4.a, cannot be reconstructed from the finite graph depicted in Fig 4.d.

c. Every FTC system generated by the DT embedding of a 2-dimensional LFPC system can be represented by a finite toroidal graph. (i.e. 2-dimensional FTC systems are considered as a subset of toroidal graphs). This implies that the topological analysis of 2-dimensional LFPC systems can be reduced to the characterization of traditional toroidal graphs embedded on a genus 1 surface.

4. Topological properties of FTC systems

In order to simplify the treatment of problems to be outlined, we introduce some definitions. Let us denote by $N_{d,k}$ the number of k-dimensional faces of FTC system $\boldsymbol{R_d}$ where k=0,1,2,…d. By definition, $N_{d,d}$ is the number of cells (polyhedra), $N_{d,0}$ is the total number of vertices, $N_{d,1}$ is the total number of edges, $N_{d,2}$ is the total number of traditional faces of cells.

The finite toroidal cellular system $\boldsymbol{R_d}$ generated by space filling polyhedra (polytopes) can be represented as

$$\boldsymbol{R_d} = \{A_{n,i} \mid i=1,2,..N_n,\ n_{min} \le n \le n_{max},\ n \in I_R\}. \qquad (5)$$

In Eq.(5), $A_{n,i}$ denotes the ith cell (d-dimensional polyhedron) with n-faces, where i= 1,2,...N_n and N_n is the total number of d-dimensional, n-faceted cells in $\boldsymbol{R_d}$. By definition, an n-faceted cell stands for a d-dimensional cell having (d-1)

dimensional faces of number n. It is supposed that $n_{min}\geq 2$ and $n_{max} > n_{min}$ are positive integers, I_R is a finite index set for n.

The total number $N_{d,d}$ of cells is $N_{d,d}=\sum N_n$ where n=2,3,... n_{max}. The fraction (or frequency) p_n of n-faceted cells is $p_n = N_n/N_{d,d}$, where $p_n>0$. Consequently, $\sum p_n =1$. For a FTC system, the mean number of (d-1) dimensional faces per cell denoted by $\langle n\rangle$ can be calculated as $\langle n\rangle = \sum np_n$. Generally, in the cell statistics, expression $\langle U(n)\rangle$ is the average value of the quantity U(n) with frequency p_n, i.e. $\langle U(n)\rangle = \sum p_n U(n)$ by definition.

Since any (d-1) dimensional face is a common face of two different neighbor cells, this implies that

$$\langle n\rangle = \sum_n np_n = \frac{2\sum_n nN_n}{N_{d,d}} = \frac{2N_{d,d-1}}{N_{d,d}} \tag{6}$$

and

$$\sum_n \sum_{k\leq n} e_{d-1}(n,k) = \sum_n \sum_{k\geq n} e_{d-1}(n,k) = N_{d,d-1} \tag{7}$$

where $N_{d,d-1}$ is the total number of (d-1) dimensional faces, and $e_{d-1}(n,k)$ is the number of the common (d-1) dimensional faces of n-faceted and k-faceted neighbor cells.

In a FTC system, vertices do not all have the same valency, consequently, we may define an average valency [r] as follows:

$$[r] = \frac{1}{N_{d,0}} \sum_r rV_r^{(d)} \tag{8}$$

where $V_r^{(d)}$ is the number of r-valent vertices in $\boldsymbol{R_d}$ and $N_{d,0} = \sum_r V_r^{(d)}$. For every FTC system we have

$$2N_{d,1} = [r]N_{d,0} = \sum_r rV_r^{(d)} \tag{9}$$

which is due to the fact, that each edge has two different ends (endvertices).

The component number of a FTC system is defined by $\Phi = \sum \mathrm{sgn}(p_n)$. It follows from the definition that $\Phi\geq 1$. On the other hand, $\Phi=1$, if and only if the FTC system is a so-called face-homogenous system which is composed only of

polyhedra with identical face numbers. It should be noted that there exist face-homogenous LFPC systems including combinatorially different cells (i.e. topologically non-equivalent polyhedra) with identical face numbers. (The simplest 3-dimensional LFPC system of such type is composed of two combinatorially different 5-sided polyhedra.)

4.1 Euler-equation for FTC systems

It is has been shown, that the traditional Euler-formula can be extended to the topological description of FTC systems [7, 9-11]. This modified Euler-equation, which valid even for a d-dimensional FTC system can be formulated as follows:

For an arbitrary FTC system $\boldsymbol{R}_{\mathbf{d}}$ where all the k-dimensional faces are topologically equivalent to a k-dimensional sphere, the equality

$$\chi\left(\mathbf{R}_{\mathbf{d}}\right)=\sum_{k=0}^{d}(-1)^{k} N_{d,k}=0 \tag{10}$$

is valid. In Eq.(10), $\chi(\boldsymbol{R}_{\mathbf{d}})$ is the Euler-characteristic of the finite toroidal cellular system $\boldsymbol{R}_{\mathbf{d}}$. Particularly, for the case of d=2, we have

$$N_{2,2}-N_{2,1}+N_{2,0}=0 \tag{11}$$

while for the case of d=3,

$$-N_{3,3}+N_{3,2}-N_{3,1}+N_{3,0}=0 \tag{12}$$

yields.

Because the unit domain $\boldsymbol{\Pi}_{\mathbf{d,U}}$ representing the corresponding LFPC system has a minimum volume, it follows that the total numbers of k-dimensional faces in $\boldsymbol{R}_{\mathbf{d}}$ (k=0,1,2,…d), i.e. quantities $N_{d,k}$ in Eqs. (10-12) are uniquely defined positive integers.

For the 2-dimensional case, identity (11) coincides with Euler's theorem for the torus [7,9]. For the 3-dimensional case, Eq.(12) has been proven by Kinsey [10], who verified that if $\boldsymbol{R}_{\mathbf{3}}$ is a compact connected 3-manifold without a boundary then $\chi(\boldsymbol{R}_{\mathbf{3}}) = 0$. The proof of the general case is based on the following concept: Considering the Euler-characteristic of a d-dimensional torus, we argue as follows: The d-dimensional torus can be represented as the direct product of d circles (meaning d circular arcs). Since the Euler-characteristic is multiplicative with respect to direct products and the Euler-characteristic of a circle is zero, this implies that the Euler-characteristic of a d-dimensional torus is zero, as well. (See Exercise B4 on page 205 in Ref. [11]).

4.2 Cell coronas

The analysis of local topological properties can be traced back to the evaluation of the correspondences between the individual cells and their first neighbor cells. Cells A and B are called adjacent (neighbors) if they have common (d-1) dimensional faces. The cell corona C(A) of a cell A in $\boldsymbol{R}_{\mathbf{d}}$ is the union of neighbor cells of A. According to this definition, cell A is not included in C(A).

FTC systems can also be characterized on the basis of the topological properties of their cell coronas. For this purpose, we define the corona frequency vector $\mathbf{f}_{\mathbf{A}}$ (CF-vector) of cell A included in $\boldsymbol{R}_{\mathbf{d}}$ as follows:

$$\mathbf{f}_{\mathbf{A}} = \left(f_2^{(A)}, f_3^{(A)}, ... f_k^{(A)} .... f_{n_{max}}^{(A)}\right) \tag{13}$$

where component $f_k^{(A)}$ is the number of (d-1) dimensional, k-faceted cells in C(A), and index n_{max} denotes the maximum (d-1) dimensional face number of cells included in $\boldsymbol{R}_{\mathbf{d}}$. It is obvious that for any k and $f_k^{(A)}$ relationships $0 \leq f_k^{(A)} \leq n_{max}$ and $n_{min}=2 \leq k \leq n_{max}$ are valid, and $f_k^{(A)} = 0$ if and only if, there is no k-faceted neighbor cell in C(A). It is clear that, if A is an n-faceted cell, then the sum of components of $\mathbf{f}_{\mathbf{A}}$ is equal to n.

Consider two n-faceted cells A_n and B_n characterized by their corresponding CF-vectors denoted by $\mathbf{f}_{\mathbf{A,n}}$ and $\mathbf{f}_{\mathbf{B,n}}$. Cells A_n and B_n are called topologically similar, if $\mathbf{f}_{\mathbf{A,n}} \equiv \mathbf{f}_{\mathbf{B,n}}$ is fulfilled. As can be stated, this topological similarity is an equivalence relation by which all the cells of a FTC system can be classified into disjoint subsets.

This implies that all the topologically similar n-faceted cells denoted by $A_{n,j}^{(1)}, A_{n,j}^{(2)}, ..., A_{n,j}^{(R_{n,j})}$ are the elements of the same configuration set $\boldsymbol{R}_{\mathbf{n,j}}$ defined as

$$\boldsymbol{R}_{\mathbf{n,j}} = \left\{A_{n,j}^{(1)}, A_{n,j}^{(2)}, ..., A_{n,j}^{(R_{n,j})}\right\} \tag{14}$$

where $R_{n,j}$ is the number of topologically similar n-faceted cells in $\boldsymbol{R}_{\mathbf{n,j}}$ (j=1,2,…J(n)). It follows that $\boldsymbol{R}_{\mathbf{d}}$ can be described as a union of disjoint subsets

$$\mathbf{R}_{\mathbf{d}} = \bigcup_{n} \bigcup_{j=1}^{J(n)} \mathbf{R}_{\mathbf{n,j}} \tag{15}$$

where J(n) stands for the number of configuration sets including topologically similar, n-faceted cells. It is obvious that cells belonging to $\boldsymbol{R}_{\mathbf{n,j}}$ is characterized by

the same FC-vector $\mathbf{f}_{\mathbf{R_{n,j}}}$. Let us denote by $p_{n,j}$ the fraction of topologically similar n-faceted cells included in $\boldsymbol{R}_{\mathbf{n,j}}$. Because $p_{n,j}= R_{n,j}/N_{d,d}$ it follows that

$$\sum_{n}\sum_{j=1}^{J(n)} p_{n,j} = \sum_{n} p_{n} = 1 \tag{16}$$

It is easy to see that $p_{n,j}$ and $\mathbf{f}_{\mathbf{R_{n,j}}}$ are unambiguously defined quantities which are independent of the particular choice of the unit domain of the LFPC system. It follows that the total number J of possible configuration sets $\boldsymbol{R}_{\mathbf{n,j}}$ can be calculated as

$$J = \sum_{n} J(n) = \sum_{n}\sum_{j} \mathrm{sgn}(p_{n,j}) \tag{17}$$

It is obvious that for any FTC system inequality $J \geq \Phi$ is fulfilled. This means that the total number of possible configuration sets is not less than the component number Φ of the FTC system. The quotient $\varphi=\Phi/J \leq 1$ which is called the complexity index of the cellular system, gives information on the fraction of topologically distinct cell coronas in the LFPC and the corresponding FTC system.

4.3 Face-coordination number

The face-coordination number m_A of an arbitrary n-faceted cell A belonging to the configuration set $\boldsymbol{R}_{n,j}$ is defined as

$$m_A = \frac{1}{n}\sum_{k} k f_k^{(R_{n,j})} \tag{18}$$

where $f_k^{(R_{n,j})}$ is kth component of the CF-vector $\mathbf{f}_{\mathbf{R_{n,j}}}$.

The face-coordination number m_A is the mean number of (d-1) dimensional faces of the neighbors of A. It should be emphasized that m_A is a local topological parameter, which gives some information on the arrangement of the cells included in the cell-corona. For the FTC system $\boldsymbol{R}_{\mathbf{d}}$ which is composed of cells $A_{n,i}$ ($i=1,2,..N_n$), the mean face-coordination number m(n) of n-faceted cells is defined as

$$m(n) = \frac{1}{N_n}\sum_{i=1}^{N_n} m_{A_{n,i}} \tag{19}$$

where $m_{A_{n,i}}$ is the face coordination number of cell $A_{n,i}$.

Knowing the set of FC-vectors $\mathbf{f}_{\mathbf{R_{n,j}}}$ and the corresponding fractions $p_{n,j}$ of topologically similar cells, the mean face-coordination number m(n) of n-faceted cells can be calculated as

$$m(n) = \frac{1}{np_n} \sum_{j=1}^{J(n)} p_{n,j} \left\{ \sum_k k f_k^{(R_{n,j})} \right\} \tag{20}$$

Starting with Eqs.(19 and 20) we define the total face-coordination number $\langle m(n) \rangle$ of $\boldsymbol{R}_\mathbf{d}$ as follows

$$\langle m(n) \rangle = \sum_n p_n m(n) = \sum_n \frac{1}{n} \sum_{j=1}^{J(n)} p_{n,j} \left\{ \sum_k k f_k^{(R_{n,j})} \right\} \tag{21}$$

It is conjectured that for all FTC systems inequality $\langle m(n) \rangle \geq \langle n \rangle$ holds, and $\langle m(n) \rangle = \langle n \rangle$ if and only if, the cellular system is a face-homogenous system including cells with identical face numbers only (i.e. $\Phi = 1$ is fulfilled).

4.4 Neighborhood coefficients

Now, let us define quantities denoted by H(n,k) as

$$H(n,k) = \sum_{j=1}^{J(n)} p_{n,j} f_k^{(R_{n,j})} \tag{22}$$

where $n_{min} \leq n,k \leq n_{max}$. Quantities H(n,k) are called the neighborhood coefficients of the FTC system. The neighborhood coefficients are non-negative numbers, which have a special property of symmetry

$$H(n,k) = \sum_{j=1}^{J(n)} p_{n,j} f_k^{(R_{n,j})} = \sum_{j=1}^{J(k)} p_{k,j} f_n^{(R_{k,j})} = H(k,n) \tag{23}$$

The neighborhood coefficients can be interpreted geometrically as follows:

$$H(n,k) = \begin{cases} \dfrac{1}{N_{d,d}} e_{d-1}(n,k) & \text{if} \quad n \neq k \\ \dfrac{2}{N_{d,d}} e_{d-1}(n,n) & \text{if} \quad n = k \end{cases} \tag{24}$$

where $N_{d,d}$ is the number of d-dimensional cells, and $e_{d-1}(n,k)$ is the number of the common (d-1) dimensional faces of n-faceted and k-faceted neighbor cells.

Especially, for the case of d=2, we have

$$H(n,k)=\begin{cases}\dfrac{1}{N_{2,2}}e_1(n,k) & \text{if} \quad n\neq k\\ \\ \dfrac{2}{N_{2,2}}e_1(n,n) & \text{if} \quad n=k\end{cases} \tag{25}$$

where $N_{2,2}$ is the number of 2-dimensional cells (polygons), and $e_1(n,k)$ is the number of the common edges (i.e. 1-dimensional faces) of n-sided and k-sided neighbor cells.

For the case of d=3,

$$H(n,k)=\begin{cases}\dfrac{1}{N_{3,3}}e_2(n,k) & \text{if} \quad n\neq k\\ \\ \dfrac{2}{N_{3,3}}e_2(n,n) & \text{if} \quad n=k\end{cases} \tag{26}$$

where $N_{3,3}$ is the number of 3-dimensional cells (polyhedra) and $e_2(n,k)$ is the number of the common 2-dimensional faces of n-faceted and k-faceted neighbor polyhedra.

It is easy to verify, that for quantities H(n,k) the following relationships are valid:

$$p_n=\frac{1}{n}\sum_k H(n,k)=\frac{1}{n}\sum_k H(k,n) \tag{27}$$

$$\sum_n\left\{\sum_k H(n,k)\right\}^z=\sum_n p_n^z n^z \tag{28}$$

$$\sum_n\sum_k k^z H(n,k)=\sum_n n^z\sum_k H(n,k)=\sum_n p_n n^{z+1}=\left\langle n^{z+1}\right\rangle \tag{29}$$

where z is an arbitrary integer. Additionally, from Eq.(6), identity

$$N_{d,d}\sum_n\sum_k H(n,k)=N_{d,d}\langle n\rangle=2N_{d,d-1} \tag{30}$$

yields. For the case of d=2 we have

$$N_{2,2}\sum_{n}\sum_{k}H(n,k)=N_{2,2}\langle n\rangle=2N_{2,1}=2\sum_{n}\sum_{k\le n}e_1(n,k) \qquad (31)$$

where $N_{2,1}$ is the total number of edges (i.e. 1-dimensional faces) and $\langle n\rangle$ is the mean number of edges per cell in $\boldsymbol{R_2}$. For the case of d=3

$$N_{3,3}\sum_{n}\sum_{k}H(n,k)=N_{3,3}\langle n\rangle=2N_{3,2}=2\sum_{n}\sum_{k\le n}e_2(n,k) \qquad (32)$$

yields, where $N_{3,2}$ is the total number of 2-d faces and $\langle n\rangle$ is the mean number of faces per cell in $\boldsymbol{R_3}$. As an example of application of these ideas, we consider the 3-dimensional, periodic Weaire-Phelan cellular system shown in **Fig.1**. This 2-component and 4-valent polyhedral system (i.e. $\Phi=2$, R=4) consisting of 12- and 14-sided polyhedra is characterized by the following topological quantities: $p_{12}=1/4$, $p_{14}=3/4$, $\langle n\rangle=27/2=13.5$, $\langle n^2\rangle=183$, $\varphi=\Phi/J=2/3=0.667$, H(12,12)=1, H(12,14) = H(14,12)=2 and H(14,14)=17/2=8.5.

5. A fundamental property of LFPC and FTC systems

Neighborhood coefficients H(n,k) play a key role in the topological characterization of LFPC systems. In the following a fundamental property of LFPC and FTC systems will be presented which can be formulated in the following statements:

On the one hand

$$\langle n^{z+1}\rangle=\frac{\langle n\rangle}{2N_{d,d-1}}\sum_{n}\sum_{k\le n}\left(n^z+k^z\right)e_{d-1}(n,k) \qquad (33)$$

on the other hand

$$\langle n^{z+1}\rangle=\langle nm(z,n)\rangle \qquad (34)$$

where z is an arbitrary integer, and

$$m(z,n)=\frac{1}{np_n}\sum_{j=1}^{J(n)}p_{n,j}\left\{\sum_{k}k^z f_k^{(R_{n,j})}\right\} \qquad (35)$$

by definition. As it can be stated, Eq. (35) is the generalization of Eq.(20). As a special case, when z=1, from Eq.(35) we obtain the mean face coordination number m(n) of n-faceted cells which is defined by Eq.(20). Consequently, identity m(n)=m(1,n) is fulfilled.

Proof of Eq. (33) is based on the following concept. Starting with Eqs.(24 and 29), we have

$$\langle n^{z+1}\rangle = \sum_n \sum_k k^z H(n,k) =$$

$$\sum_n n^z H(n,n) + \sum_{n\neq k}\left\{\sum_k k^z H(n,k)\right\} =$$

$$\frac{2}{N_{d,d}}\sum_n n^z e_{d-1}(n,n) + \frac{1}{N_{d,d}}\sum_{n\neq k}\left\{\sum_k k^z e_{d-1}(n,k)\right\} =$$

$$\frac{1}{N_{d,d}}\sum_n e_{d-1}(n,n)\left\{n^z + n^z\right\} +$$

$$\frac{1}{N_{d,d}}\left\{\sum_{\substack{n,k\\ n>k}} n^z e_{d-1}(n,k) + \sum_{\substack{n,k\\ n>k}} k^z e_{d-1}(n,k)\right\} =$$

$$\frac{1}{N_{d,d}}\sum_{\substack{n,k\\ n\geq k}} (n^z + k^z) e_{d-1}(n,k) \tag{36}$$

Additionally, from Eq. (30) it follows

$$N_{d,d} = \frac{2N_{d,d-1}}{\langle n\rangle} \tag{37}$$

Substituting Eq.(37) into Eq.(36) we have

$$\langle n^{z+1}\rangle = \langle n\rangle \sum_n \sum_{k\leq n} \frac{e_{d-1}(n,k)}{N_{d,d-1}}\left(\frac{n^z + k^z}{2}\right) \tag{38}$$

It is important to note that Eq.(38) can be interpreted geometrically as follows: Let us denote by $q(n,k)=e_{d-1}(n,k)/N_{d,d-1}$ the relative frequency of the common faces of n-faceted and k-faceted neighbor cells, for which $\sum q(n,k) = 1$. Additionally, let us define quantities denoted by $w(z,n,k)= (n^z + k^z)/2$, which are considered as

positive weights belonging to the (d-1) dimensional common face of n- and k-faceted neighbor cells. Now, Eq.(38) can be rewritten in the form

$$\langle n^{z+1}\rangle = \langle n\rangle \sum_{n}\sum_{k\le n} q(n,k)w(z,n,k) \tag{39}$$

It is worth noting, when z = -1, from Eqs.(37 and 38) the identity

$$N_{d,d} = \sum_{n}\sum_{k\le n} e_{d-1}(n,k)\left(\frac{1}{n}+\frac{1}{k}\right) \tag{40}$$

yields.

The second statement represented by Eq.(34) can be proved as follow: By using Eq.(35) and Eq.(23) incorporating the definitions of quantities m(z,n) and H(n,k), we have

$$\langle nm(z,n) = \sum_{n}\sum_{j=1}^{J(n)} p_{n,j}\left\{\sum_{k} k^{z} f_{k}^{(R_{n,j})}\right\} =$$

$$\sum_{n}\left\{\sum_{k} k^{z}\left\{\sum_{j=1}^{J(n)} p_{n,j} f_{k}^{(R_{n,j})}\right\}\right\} = \sum_{n}\left\{\sum_{k} k^{z} H(n,k)\right\} = \langle n^{z+1}\rangle \tag{41}$$

In particular cases, when z =1, from Eq.(41) we obtain the well-known identity formulated as $\langle nm(n)\rangle = \langle n^2\rangle$ which were considered by Weaire and Fortes [2,3] for random 2-d cellular systems, and by Fortes for random 3-d cellular systems [4].

In the following it will be demonstrated that the general concept used for the topological description of locally finite periodical cellular systems can be efficiently applicable to the structural characterization of fullerene solids represented by finite cellular surface systems.

6. Cellular fullerenes

The discovery of fullerene molecules and related forms of carbon such as nanotubes has generated an explosion of activity in physics, chemistry and material science. As it is known, the topological properties of fullerenes play a key role in a classification of possible fullerene structures and in predicting their various physical and chemical behaviors.

In chemistry, the traditional definition is that a fullerene is an all-carbon molecule in which the atoms are arranged on a pseudospherical framework made up entirely of hexagons and pentagons. Based on the concept outlined in Refs. [12-14], define a fullerene in the wider sense as follows: A fullerene is considered as a simple finite cellular system (SFC system) defined on an unbounded, closed and oriented surface, and composed of a finite set of combinatorial polygons (called cells), where cells are simply connected regions and all common edges are shared only by two different neighbor cells. Fullerenes of such types will be referred to as cellular fullerenes. According to this general definition, the closed nonotubes with negative curvature and the so-called onion-like structures are also considered as fullerenes [13,14]. Taking into consideration the decisive role of the Euler characteristic (χ) in the topological analysis of unbounded, closed and oriented surfaces, cellular fullerenes with $\chi=2$ are called spherical, while cellular fullerenes with $\chi=0$ are called toroidal fullerenes.

6.1 Non-polyhedral spherical fullerenes

Cellular spherical fullerenes generated by the tessellation of the surface of the unit sphere can be classified into two classes. Spherical fullerenes represented by convex polyhedra are called polyhedral fullerenes, while the others, which cannot be represented by convex polyhedra, are called non-polyhedral fullerenes. It should be noted that, the Schlegel diagram of a polyhedral fullerene is considered as a polyhedral graph. According to the Steinitz's theorem, a finite graph is polyhedral if and only if it is planar and 3-connected [16]. This implies that the Schlegel diagram of a non-polyhedral spherical fullerene is represented by a 2-connected graph. It is important to note, that among the spherical fullerenes there exist several topologically distinct isomers, which can be of polyhedral and non-polyhedral types.

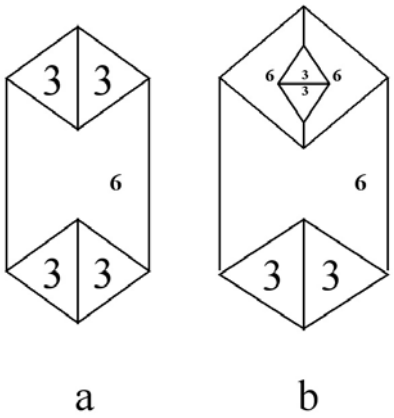

Fig.5 Schlegel diagrams of non-polyhedral, trivalent fullerenes: (a) a generalized triangular $\mathbf{T_{8,is}}$ fullerene with 8 vertices, (b) a generalized triangular $\mathbf{T_{12,is}}$ fullerene with 12 vertices

Deza et al. investigated some special types of polyhedral fullerenes, namely, the so-called triangular fullerenes composed of triangles and hexagons only [15]. A triangular fullerene is defined as a simple polyhedron with trivalent vertices, for which the k vertices are arranged in 4 triangles and (k/2-2) hexagons (and 3k/2 edges). Triangular fullerenes denoted by $\mathbf{T_k}$ can be constructed for all $k \equiv 0 \pmod 4$ except k=8. Examples of such polyhedra are the tetrahedron $\mathbf{T_4}$, the truncated tetrahedron $\mathbf{T_{12}}$ and the chamfered tetrahedron $\mathbf{T_{16}}$ [15]. By extending the definition of triangular fullerenes we can construct spherical and trivalent isomers, which are of non-polyhedral types. In **Fig.5** the corresponding Schlegel diagrams of two non-polyhedral triangular fullerenes denoted by $\mathbf{T_{8,is}}$ and $\mathbf{T_{12,is}}$ are shown. It is worth noting that $\mathbf{T_{8,is}}$ is the smallest non-polyhedral trivalent fullerene because $\mathbf{T_{8,is}}$ has no isomers of polyhedral types.

6.2 Global topological properties of cellular fullerenes

In a SFC system, the total number E of edges is related to the total number N_t of cells, the number V of vertices, the average valency [r] and the mean number of sides per cell $\langle n \rangle$

$$2E = \sum_n nN_n = \langle n \rangle N_t = \sum_r rV_r = [r]V \qquad (42)$$

where N_n is the number of n-sided polygons. The number V of vertices is $V = \sum V_r$ where V_r is the number of r-valent vertices, the total number N_t of cells

(polygons) is $N_t = \sum N_n$ where n=2,3,... n_{max}, and the fraction p_n of n-sided cells is $p_n = N_n/N_t$, for $p_n > 0$.

Assuming that all the cells are simply connected regions, Euler's equation can be formulated as

$$\chi = N_t - E + V = 2 - 2g \tag{43}$$

where χ is the Euler-characteristic, g is the genus of the surface [16]. The genus of the surface, which can be an arbitrary non-negative integer, is identical to the number of handles that are attached to the sphere to obtain a surface. For the sphere χ=2 and g=0, for the torus (donut) χ= 0 and g=1, for the double torus, χ = - 2 and g=2, for the triple torus, χ = -4 and g=3, respectively. It is worth noting that identity (43) is a possible generalization of Eq.(11), because for the torus (where equalities χ=0 and g=1 are fulfilled), from Eq.(43) we obtain Eq.(11) as a special case. Taking into consideration, that for a SFC system equalities $\langle n \rangle = 2E/N_t$ and $[r] = 2E/V$ are fulfilled, from Eqs.(42 and 43), we have

$$\frac{1}{[r]} + \frac{1}{\langle n \rangle} = \frac{1}{2} + \frac{1-g}{E} = \frac{1}{2} + \frac{\chi}{2E}. \tag{44}$$

Additionally, from Eqs. (42 - 44) it follows

$$\langle n \rangle = \frac{2[r]}{[r]-2}\left\{1 - \frac{\chi}{N_t}\right\} = 2\frac{1 - \frac{\chi}{N_t}}{1 - \frac{V}{E}} \tag{45}$$

$$N_t = \chi + V([r]-2)/2 \tag{46}$$

and

$$\frac{1}{V}\sum_r (r-2)V_r = \sum_r (r-2)u_r = 2\frac{N_t - \chi}{V} = 2\frac{E-V}{V} \tag{47}$$

where $u_r = V_r/V$ is the fraction of r-valent vertices, for which $\sum u_r = 1$ and $\sum r u_r = [r]$ are fulfilled. An immediate consequence of Eq.(45) is that for trivalent SFC systems, equality $\langle n \rangle = 6(1-\chi/N_t) = 6-12\chi/(2\chi+V)$ is valid. Depending on the particular choice of the Euler–characteristic χ, as particular cases, we get $\langle n \rangle < 6$ for a sphere (case χ=2), $\langle n \rangle = 6$ for a torus (case χ=0) and $\langle n \rangle > 6$ for a double torus (case χ=-2), respectively.

6.3 Local topological properties of cellular fullerenes

First of all, it is important to emphasize that general formulae derived for d-dimensional LFPC systems (see formulae given by Eqs.(6 - 41)) can be applied to arbitrary fullerenes represented by simple finite cellular systems. It is easy to see that the fundamental identities given by Eqs.(33 and 34) remain valid for any SFC system (i.e. for cellular fullerenes).

In the following, by introducing the notion of the so-called vertex corona, we will demonstrate that the vertex corona distribution can be efficiently used to the local topological characterization of regular (R-valent) cellular fullerenes represented by SFC systems.

In a SFC system, cells A and B are called diagonally adjacent (diagonal neighbors) if they have a common vertex X. Vertex corona $C_V(X)$ of an arbitrary vertex X is defined as a union of diagonal neighbor cells having a common vertex X. For a finite cellular system characterized by the sequence of vertices X_k (k =1,2, …V)

$$C_V(X_k) = \bigcup_j A_j(X_k) \tag{48}$$

where X_k is a common vertex of cells $A_j(X_k)$.

Vertex corona distribution of a cellular fullerene represented by a regular SFC system has an interesting property. Consider a finite cellular system, where $X_{r,k}$ denotes the kth and r-valent vertex, and define the topological quantity

$$M_v = \frac{1}{V}\sum_{k=1}^{V} M(r,k) \tag{49}$$

where M(r,k) stands for the mean number of sides of cells in $C_V(X_{r,k})$ for k = 1,2,…V. The local topological parameter M(r,k) is called the vertex coordination number of $X_{r,k}$ while M_v is said to be the total vertex coordination number of the FTC system.

Now, we will verify that for regular, R-valent FTC systems (i.e. cellular fullerenes), identity

$$\langle n^2 \rangle = \langle n \rangle M_v \tag{50}$$

is valid. Proof of Eq. (50) is based on the following considerations: Let us denote by $n(B_j^{(k)})$ the side number of cell $B_j^{(k)}$ belonging to the vertex corona $C_V(X_{R,k})$, where k = 1,2,…V and j=1,2,…R. It follows that

$$M(R,k) = \frac{1}{R}\left\{n(B_1^{(k)}) + n(B_2^{(k)}) + ...n(B_j^{(k)}),... + n(B_R^{(k)})\right\} \tag{51}$$

Starting with Eq.(51), we have

$$M_v = \frac{1}{V}\sum_{k=1}^{V} M(R,k) = \frac{1}{VR}\sum_{k=1}^{V}\sum_{j=1}^{R} n(B_j^{(k)}) = \frac{1}{VR}\sum_{n} n^2 N_n =$$

$$= \frac{N_t}{VR}\sum_{n} n^2 p_n = \frac{N_t}{2E}\langle n^2\rangle = \frac{\langle n^2\rangle}{\langle n\rangle} \qquad (52)$$

It is easy to see that formula (50) can be generalized as follows: If z is an arbitrary integer, then identity

$$\langle n^{z+1}\rangle = \langle n\rangle M_v(z) \qquad (53)$$

is valid for regular SFC systems, where

$$M_v(z) = \frac{1}{V}\sum_{k=1}^{V} M(R,k,z) \qquad (54)$$

and

$$M(R,k,z) = \frac{1}{R}\left\{n^z(B_1^{(k)}) + n^z(B_2^{(k)}) + ,... + n^z(B_R^{(k)})\right\} \qquad (55)$$

by definition. As it can be stated, when z = 1, this implies that Eq. (53) is simplified to Eq. (50). This is due to the fact, in the case of z=1, it follows that M(R,k,1)= M(R,k) and $M_V(1) = M_V$, respectively.

For trivalent and 2-component cellular fullerenes, (i.e. for the case of Φ=2 and R=3), which include α-sided and β-sided cells with frequencies p_α and $p_\beta = 1- p_\alpha$ (where $\alpha<\beta$), there exist only four possible types of vertex coronas denoted by $C_{\alpha,\alpha,\alpha}$, $C_{\alpha,\alpha,\beta}$, $C_{\alpha,\beta,\beta}$ and $C_{\beta,\beta,\beta}$ respectively. This implies that in this particular case, Eq.(50) can be reduced to the form

$$M_v = s_1 M_1 + s_2 M_2 + s_3 M_3 + s_4 M_4 = \frac{\langle n^2\rangle}{\langle n\rangle} \qquad (56)$$

where $M_1=(\alpha+\alpha+\alpha)/3$, $M_2=(\alpha+\alpha+\beta)/3$, $M_3=(\alpha+\beta+\beta)/3$ and $M_4 =(\beta+\beta+\beta)/3$ are the vertex coordination numbers of the four possible types of vertex coronas, and s_i (i=1,2,3,4) are the corresponding relative fractions of the vertex coronas, for which $\sum s_i = 1$ holds. Using identity (56) facilitates the computation of vertex fractions s_i (i=1,2,3,4), which are topological invariants. (For example, if quantities s_1 and s_2 are known, then s_3 and s_4 can be directly calculated.)

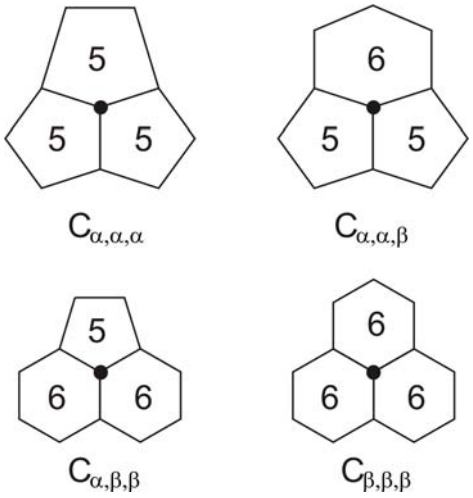

Fig.6 The four possible vertex coronas in a 2-component, trivalent fullerene (case α=5 and β=6).

6.4 Application: Topological characterization of C_{60} fullerenes

As we have mentioned previously, the analysis of the distribution of vertex coronas of different types plays a significant role in algorithms for the perception and classification of topological properties of fullerenes. Balaban et al. have used this concept in order to classify the C_{60} isomers on the basis of topological properties of their vertex coronas [17]. Since C_{60} fullerene isomers are composed of 12 pentagons and 20 hexagons, in this particular case, we have: α=5, β=6, and p_5=12/32, p_6=20/32, $\langle n\rangle$=45/8=5.625, $\langle n^2\rangle$=255/8 and M_V=17/3=5.667. The corresponding vertex coordination numbers are: M_1=15/3, M_2=16/3, M_3=17/3 and M_4 =18/3. As Balaban et al. [17] pointed out, the 1812 structural isomers of C_{60} fullerenes could be partitioned into 42 equivalence classes (subclasses) on the basis of the four types of vertex coronas $C_{5,5,5}$, $C_{5,5,6}$, $C_{5,6,6}$ and $C_{6,6,6}$ which are illustrated in **Fig. 6**.

To characterize the local topological structure of cellular fullerenes, we defined the topological descriptor IS calculated on the basis of the neighborhood coefficients:

$$IS = \sum_{n} H(n,n) \qquad (57)$$

The topological descriptor IS which is called the isolation index can be simply computed for C_{60} isomers

$$IS = \langle n \rangle - 2H(5,6) = \langle n \rangle - \frac{2V}{N_t}\left(1 - s_1 - s_4\right) = \frac{45}{8} - \frac{15}{4}\left(s_2 + s_3\right) \geq \frac{15}{8} \quad (58)$$

where s_i (i=1,2,3,4) are the relative fractions of the corresponding vertex coronas. (See **Fig.6**.) Based on the calculated results the following conclusions can be drawn:

By using the isolation index the 1812 C_{60} isomers can be partitioned into 18 subclasses. Calculated values of isolation index IS are in the interval 1.875 to 4.375.

The buckminster-fullerene denoted by C60B (containing 12 isolated pentagons) is the sole isomer which is characterized by the minimum value of IS (namely IS=15/8 =1.875). The computed neighborhood coefficients are: H(5,5) = 0, H(5,6) = H(6,5) = H(6,6) =15/8). It should be noted that it is supposed that fullerene structures with isolated pentagons are likely to be more stable than structures containing fused five-membered rings [18].

On the other hand, we found that the maximum value of IS belongs to C60W isomer (IS= 4.375). (See the corresponding Schlegel diagram of C60W shown in Fig.1 in Ref.[17]). It is important to emphasize that C60W is judged to be the least stable C_{60} isomer [17], for which the corresponding neighborhood coefficients are: H(5,5) = 10/8, H(5,6) = H(6,5) = 5/8 and H(6,6) =25/8.

We have also observed that the discriminating performance of the topological index IS is determined (and limited) primarily by the local neighborhood structure of the cellular system. For cellular systems characterized by a topologically similar first neighbor structure, the neighborhood dependent isolation index has only a limited ability for discrimination. The main advantage of using the isolation index lies in the fact that IS can be generally applied to the topological characterization of any cellular system, not only fullerene-like but also arbitrary infinite periodical cellular structures.

7. Summary and conclusions

A general method has been developed to characterize and compare infinite and finite cellular systems on the basis of quantitative topological criteria. First, we analyzed the global and local topological properties of infinite periodic cellular structures, and then the theoretical results obtained have been adapted to the local topological characterization of 2-dimensional finite cellular surface systems. The general concept of this new approach is based on the use of the so-called double toroidal embedding (DT embedding) by which a finite cellular system defined on a torus can be generated from an infinite periodic cellular system.

As a result of performing a DT embedding, so-called neighborhood coefficients can be generated. The neighborhood coefficients H(n,k) are simple scalar topological invariants, by which the local topological structure of cellular systems

can be quantitatively evaluated and compared. Moreover, by investigating the relationship between the neighborhood coefficients and other local topological quantities, we have verified that the validity of the Weaire-Fortes identity (playing a key role in the topological description of 2-dimensional random cellular patterns), could be extended to infinite periodic cellular systems and 2-d finite cellular surface systems (i.e. generalized fullerene-like structures). It has been also shown that the traditional definition of fullerenes can be generalized by introducing the notion of the cellular fullerene, which is considered as a finite cellular system defined on a 2-d unbounded, closed and orientable surface.

From the previous considerations it follows that the fundamental Eqs. (33 and 34) remain valid not only for cellular systems consisting of combinatorial polyhedra (which are topologically equivalent to a d-dimensional ball), but

- for finite cellular systems defined on an unbounded, closed and orientable surface (sphere, torus, double torus , etc.),
- for infinite triply periodic 3-d surface systems, in which the internal surface represented by “infinite tunnels” is composed of polygons [19]. (Typical examples are the so-called zeolitic structures [20]),
- for all “pseudo-random” cellular systems which are artificially generated by the tessellation of the d-dimensional unit cube using periodic boundary conditions. Due to the periodic boundary extension, these pseudo-random structures are also considered as infinite periodic cellular systems. A well-known example is the computer simulation of the Poisson Voronoi cells where the periodic boundary condition is used to avoid edge effects [1, 21].

Finally, it should be emphasized that Eqs. (33 and 34) remain valid for such cases when the space-filling polyhedra are not equivalent topologically to d-dimensional balls, provided that the cellular system is generated from a finite set of d-dimensional cells with (d-1)-dimensional faces in such a way that all common faces are shared by two different neighboring cells.

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