Polygonal Tiling of Some Surfaces Containing Fullerene molecules

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ABSTRACT. A tiling of a surface is a decomposition of the surface into pieces, i.e. tiles, which cover it without gaps or overlaps. In this paper some special polygonal tiling of sphere, ellipsoid, cylinder, and torus as the most abundant shapes of fullerenes are investigated.

Keywords: Euler characteristic, fullerene, polygonal tiling.

1. INTRODUCTION

Fullerenes are a family of carbon allotropes which composed entirely of carbon, in the form of a sphere, ellipsoid, cylinder, or tube. The structure of fullerenes is composed of hexagonal, pentagonal or sometimes heptagonal and octagonal rings [1, 2, 3]. Other geometric shapes such as square and triangles can be found in the structure of fullerenes [4]. Some people study the structure of fullerene by graph theory [5, 6, 7]. We consider fullerenes as a polyhedron whose vertices, edges, and faces are atoms, chemical bond, and the rings respectively. So we can investigate its structure and the number of its polygons as a tiling of a surface. On the other hand, one can regard the fullerene as a 3 regular cubic graph. We compound these two views and use the Euler characteristic as a powerful tool to compute the number of a polygon in the structure of a fullerene, and the maximum number of possibility structure. We study the surfaces sphere, ellipsoid, cylinder and torus, because they are the most abundant shapes of fullerenes. It should be noted that our argument is a mathematical investigation, not a chemical analysis.

This paper is prepared as follows. In Section 2, we introduce the Euler characteristic for polyhedrons and the d-regular edge-to-edge tiling, and state and prove some result about

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Received: September 24, 2014; Accepted: October 30, 2014.

this type of tiling. In section 3 we classify the tilings up to the type of polygons in the tiling. Section 4 gives some comments and remarks about the feature works on the concept of tiling and fullerenes.

2. EULER CHARACTERISTIC AND TILING THE SURFACES

Euler characteristic is one of the most important topological invariant (in fact a homotopy invariant) for surfaces, polyhedrons, polygons, and CW-complexes. Instead of its exact topological definition, we provide its definition for polyhedrons as we need.

Definition 1. The Euler characteristic of a polyhedron M is defined as $\chi = V - E + F$, where V, E, and F, are the number of vertices, edges, and faces in M respectively.

Two homeomorphic topological spaces have the same Euler characteristic, so in order to compute the Euler characteristic of a given surface, it is enough to compute the Euler characteristic of some polyhedron homeomorphic to it. For example since a tetrahedron and sphere are homemorphic, their Euler characteristics are equal. It is easy to see that the Euler characteristic of our desire surfaces, sphere and ellipsoid is 2, and of cylinder and torus is zero. We use this in our computations. We start by some definitions an examples.

Definition 2. An edge-to edge polygonal tiling of a surface is a covering of the entire surface by geodesics polygons, with no gaps our overlaps, such that the edge of a tile coincides entirely with the edge of a bordering tile. A tiling is said to be d-regular, if its corresponding graph is d-regular. We denote by $\left[(k_1, k_2, \dots, k_r), \left(n_{k_1}, n_{k_2}, \dots, n_{k_r}\right)\right]$ a tilling in which there is n_{k_i} numbers of k_i-gons.

Definition 3. Two d-regular edge-to-edge tiling $\left[(k_1, k_2, \dots, k_r), \left(n_{k_1}, n_{k_2}, \dots, n_{k_r}\right)\right]$ and $\left[(k_1{}', k_2{}', \dots, k_r{}'), \left(n_{k_1{}'}, n_{k_2{}'}, \dots, n_{k_r{}'}\right)\right]$ for the surface M are said to be polygonal similar if $k_i = k_i{}'$ for $i = 1, \dots, r$.

It is clear that polygonal similarity is an equivalence relation on the set of all tiling for a surface.

Notation. The equivalence class corresponds to the tiling $\left[(k_1, k_2, \dots, k_r), \left(n_{k_1}, n_{k_2}, \dots, n_{k_r}\right)\right]$ is denoted by $T(k_1, k_2, \dots, k_r)$.

Example 4. The fullerene C_{60} is a 3–regular edge-to-edge tilling for sphere containing 12 pentagons and 20 hexagons. The representation of this tiling is $[(5,6), (12,20)]$ and the corresponding equivalence class is $T(5,6)$.

Theorem 5. Let $[(k_1, k_2, \dots, k_r), (n_{k_1}, n_{k_2}, \dots, n_{k_r})]$ be a d–regular, edge–to–edge tiling for a surface with Euler characteristic χ. Then

$$\sum_{i=1}^{r} \left((2-d)k_i + 2d\right) n_{k_i} = 2\chi d. \qquad (*)$$

Proof. The number of vertices, edges, and faces are:

$$V = \frac{1}{d}\left(n_{k_1}k_1 + \cdots + n_{k_r}k_r\right),\ E = \frac{1}{2}\left(n_{k_1}k_1 + \cdots + n_{k_r}k_r\right),\ F = n_{k_1} + \cdots + n_{k_r}.$$

So,

$$\chi = \frac{1}{d}\left(n_{k_1}k_1 + \cdots + n_{k_r}k_r\right) - \frac{1}{2}\left(n_{k_1}k_1 + \cdots + n_{k_r}k_r\right) + n_{k_1} + \cdots + n_{k_r},$$

implying that

$$2\chi d = \sum_{i=1}^{r} \left((2-d)k_i + 2d\right) n_{k_i}.$$

In the rest of this paper all tiling are supposed to be 3- regular and edge-to edge as the fullerenes.

Corollary 6. For every spherical fullerene with tiling $[(k_1, k_2, \dots, k_r), (n_{k_1}, n_{k_2}, \dots, n_{k_r})]$, we have

$$\sum_{i=1}^{r} (6 - k_i) n_{k_i} = 12.$$

The same result for cylinder and torus is:

$$\sum_{i=1}^{r} (6 - k_i) n_{k_i} = 0.$$

Proof. We know that fullerenes are 3-regular tiling (d=3). In the case sphere by letting $\chi = 2$ in the equation $(*)$ we have

$$12 = \sum_{i=1}^{r} \left((2-3)k_i + 6\right) n_{k_i} = \sum_{i=1}^{r} (6 - k_i) n_{k_i}.$$

The same result for cylinder and torus is obtained by taking $\chi = 0$.

By using previous corollary one can show that in every tiling of clas $T(5{,}6)$s for sphere or ellipsoid the number of pentagons is exactly 12, since

$$12 = (6-5)n_5 + (6-6)n_6 = n_5.$$

Using a similar argument, the number of tetragons in a $T(5,6)$ tiling for sphere or ellipsoid is 6, and the number of triangles in a $T(5,6)$ tiling is 4. It is also easy to show that there is no tiling of class$T(k,6)$, $k \neq 6$, for cylinder or torus.

Theorem 7. If there exists a tiling of class $T(5,7)$ or $T(5,6,7)$ for cylinder or torus, then the number of pentagons is equal to the number of heptagons. If we have such tiling for sphere or ellipsoid, then the number of pentagons is 12 more than the number of heptagons.

***Proof*.** For cylinder and torus we have

$$0 = (6-5)n_5 + (6-6)n_6 + (6-7)n_7, \quad \Rightarrow \quad n_5 = n_7.$$

Similarly in the case of sphere and ellipsoid,

$$12 = (6-5)n_5 + (6-6)n_6 + (6-7)n_7, \quad \Rightarrow \quad n_5 = 12 + n_7.$$

Applying this technique we can compute or predict the number of some special polygons in a tiling, or determine the possibility existence of some classes of tiling. For example there is no $T(6,7)$ tiling for sphere, ellipsoid, cylinder, and torus; For sphere and ellipsoid we get to the contradiction $n_7 = -12$, while for torus and cylinder we obtain another contradiction, $n_7 = 0$.

3. CLASSIFY THE TILINGS

In this section we will go on and investigate the tiling of classes $T(k_1)$, $T(k_1,k_2)$, $T(k_1,k_2,k_3)$ and $T(k_1,k_2,k_3,k_4)$, for $k_i \in \{3,4,5,6\}$. The same argument can be done for more number namely 7, 8, etc.

3.1 Classes with One Polygon.

For a tiling of class $T(k)$ the equation $(*)$ is $(6-k)n_k = 6\chi$. The possible solutions for sphere are $k = 3,4,5$. Torus and cylinder have no tiling T(k) for $k \neq 6$. These results are presented in the following table.

	Sphere and Ellipsoid			**Cylinder and Torus**		
	Equation	n_k	Tiling	Equation	n_k	Tiling
T(3)	$3n_3 = 12$	4	tetrahedron	$3n_3 = 0$	0	----
T(4)	$2n_4 = 12$	6	cube	$2n_4 = 0$	0	----
T(5)	$n_5 = 12$	12	dodecahedron	$n_5 = 0$	0	----
T(6)	----	----	----	$0n_6 = 0$	?	?

3.2 The Classes with 2 Polygons.

By simple calculation one can see that there is no $T(k_1, k_2)$ tiling for cylinder and torus for $k_i \in \{3,4,5,6\}$, because we get the unacceptable solution $n_k = 0$ for $k = 3,4,5$. So we only can tile the sphere or ellipsoid with two types of polygons. The following table presents these tilings.

$T(k_1, k_2)$	**Sphere and Ellipsoid**		
	Equation	(n_{k_1}, n_{k_2})	The Maximum number of Tiling
T(3,4)	$3n_3 + 2n_4 = 12$	(2,3)	1
T(3,5)	$3n_3 + n_5 = 12$	(1,9), (2,6), (3,3)	3
T(3,6)	$3n_3 + 0n_6 = 12$	(4,?)	?
T(4,5)	$2n_4 + n_5 = 12$	(1,10), (2,8), (3,6), (4,4), (5,2)	5
T(4,6)	$2n_4 + 0n_6 = 12$	(6,?)	?
T(5,6)	$n_5 + 0n_6 = 12$	(12,?)	?

3.3 The Classes with 3 Polygons

Same calculation as above shows that the cylinder and torus have no $T(k_1, k_2, k_3)$ tiling. But for sphere and ellipsoid equation $(*)$ have various solutions.

$T(k_1, k_2, k_3)$	Sphere and Ellipsoid		
	Equation	$(n_{k_1}, n_{k_2}, n_{k_3})$	The Maximum number of Tiling
T(3,4,5)	$3n_3 + 2n_4 + n_5 = 12$	(1,1,7),(1,2,5),(1,3,3), (1,4,1),(2,1,4),(2,2,2), (3,1,1)	7
T(3,4,6)	$3n_3 + 2n_4 + 0n_6 = 12$	(2,3,?)	?
T(3,5,6)	$3n_3 + n_5 + 0n_6 = 12$	(1,9,?),(2,6,?),(3,3,?)	?
T(4,5,6)	$2n_4 + n_5 + 0n_6 = 12$	(1,10,?),(2,8,?),(3,6,?), (4,4,?), (5,2,?)	?

3.4 Classes with 4 Polygons

The only class with 4 types of polygons is T(3,4,5,6) with corresponding equation $3n_3 + 2n_4 + n_5 + 0n_6 = 12$. In such tiling the number of hexagons is not constant. The number of other polygons is presented in the following table.

	Sphere and Ellipsoid		
	Equation	(n_3, n_3, n_6, n_7)	The Maximum number of Tiling
T(3,4,5,6)	$3n_3 + 2n_4 + n_5 + 0n_6 = 12$	(1,1,7,?),(1,2,5,?),(1,3,3,?),(1,4,1,?),(2,1,4,?),(2,2,2,?),(3,1,1,?)	?

4. MORE COMMENTS

We only considered some fullerenes which contain triangles, squares, pentagons, and hexagons. Same argument can be done for ones that contain heptagons and octagons. In the last case the solutions for equation $(*)$ is more various. For example for the class T(3,7) the equation $3n_3 - n_7 = 12$ has infinite solutions such as (5,3), (6,6),(7,9), etc. . But whether these tilings are exist or not is another problem. This research and study can be continued to illustrate various tiling for several surfaces with arbitrary Euler characteristic.

ACKNOWLEDGEMENT. This work was partially supported by the University of Kashan under grant No. 364997/1.

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