Design and realization of macroscopic grid architectures mimicking carbon molecules

Davide Gastaldi[a] and Nicola Pugno[b]

[a] G.T.C.A. Srl , Grid Structures, Via Racconigi 19, Murello CN 12030, Italy,
gtca.murello@tin.it

[b] Politecnico di Torino, Department of Structural Engineering , Corso Duca degli Abruzzi 24, Torino 10129, Italy
nicola.pugno@polito.it

Abstract. We have developed a new geometrical approach to build some special deltahedra, which might represent nano-architectures of molecular structures, in nature commonly known as fullerenes, as well as new intriguing macro-architectures for designing innovative structures. We have realized models of these nano and macro architectures including a roof-like structure for a tennis court and educational games.

Keywords: Grid structures, deltahedra, fullerenes, biological architectures, nanotubes.

1 INTRODUCTION

Grid structures are a valuable tool for engineers and architects looking for new aesthetic forms. Reducing the consumption of raw materials to the minimum is a crucial pre-requisite in the framework of sustainable development; by definition, grid structures are highly efficient, and the mechanical characteristics of their elements are utilised to the maximum. The lightness of these structures implies both a lower environmental impact and the almost total recyclability of their elements. This paper focuses on the occupation of space from a structural point of view; it singles out new aggregations of elementary structural cells.

A polyhedron is defined as a geometric object with faces, edges and vertices. From the time of ancient Egyptian civilization, mathematicians have studied and ascribed special properties to polyhedra [1,2]. The most basic polyhedra were classified for the first time by Greek mathematicians; Plato (428-347 a.C.) pointed out that regular polyhedra were the basis of the structure of the universe. Platonic polyhedra consist of the tetrahedron, cube or hexahedron, octahedron, dodecahedron and icosahedron; each of these is composed of similar faces of regular polygons; and all the faces, edges and vertices are equivalent. Semi regular polyhedra were classified by Archimedes (287-212 a.C.). The faces of these polyhedra are regular polygons which are different one another (polygons with a different number of sides, all of them have the same length). Kepler (1571-1630), by using star polygons, built star polyhedra, which have non-convex regular polygons as faces. Later, Poinsot (1777-1859) discovered the remaining two regular star polyhedra. In recent years important works were carry out by Coxeter [3].

Geodetic domes are a relevant meeting point between polyhedra and architectural forms. The dome planned by Bauersfeld in 1922, with a slightly triangular grid, is the first accidental example of geodetic dome. Other examples of what we now commonly call space grids were developed by Bell (1847-1922), by Le Ricolais (1894-1977) and by Mengeringhausen respectively in the United States of America, in France and in Germany. However, it was Fuller [4] who actually studied the geometric decomposition of regular polyhedra. In 1985. Curl, Kroto and Smalley [5] discovered a molecule made of 60 atoms of carbon with 20 hexagons and 12 pentagons, whose shape was similar to a soccer ball. Given its shape and the domes drawn by Fuller, it was named fullerene, a tribute to him (Fig. 1).
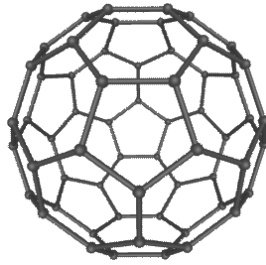
Fig. 1. The C60 fullerene.

This finding paved the way to new directions in the research on carbon - based molecular structures; a new family of carbon allotropes in the form of hollow sphere, ellipsoid, tube or plane was uncovered. Spherical fullerenes are also called buckyballs, and cylindrical ones are called carbon nanotube. Graphene is an example of a planar fullerene sheet. Fullerenes are similar in structure to graphite, which is composed of a sheet of linked hexagonal rings, but may also contain pentagonal (or sometimes heptagonal) rings that would prevent a sheet from being planar. From an architectural point of view, it is important to introduce the "tripod" concept, which allows for the interaction of the *nano* and *macro* dimensions. The tripod at the nano level can be considered as *sp*2-hybridized atom with three bonds 120° equally distributed. Again from an architectural point of view, the tripod-like element is inscribed within a equilateral triangle, with its three free ends laying on the medial point of each side of the triangle (Fig. 2). This statement will allow for the study of the forms we will realize as deltahedra.
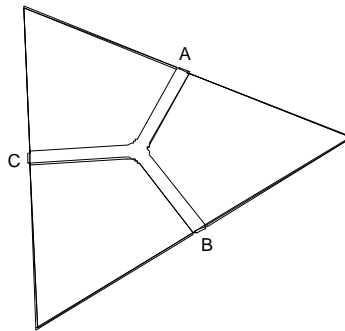

Fig. 2. The reference tripod element.

2 DELTAHEDRA

In this paper we focus attention on deltahedra, that is polyhedra whose faces are all equilateral triangles. All the deltahedra we consider are simply connected and the Euler characteristic is equal to two, i.e.:

$$\chi = V - E + F = 2 \quad , \tag{1}$$

where V are the number of vertices, E of edges and F of faces.

The geometry of spatial structures comprises fundamental information about the load bearing behaviour. In a three-dimensional space structure, it is a necessary condition for stability, known as the extended Maxwell's rule [6], is:

$$3j - b - c = m - s \ , \tag{2}$$

where the numbers j,b,c,m,s are the numbers respectively of frictionless joints, bars, kinematical constraints, internal mechanisms (joint displacement without bar extension) and states of self-stress (bar tensions in the absence of load).

For a statically determined ($c = 6$) stable space frame, without internal mechanisms and states of self-stress ($m = 0, s = 0$):

$$3j - b - 6 = 0 \ . \tag{3}$$

We suppose that exists a geometrical-physical coincidence between vertices and joints and between edges and bars; so we can use the extended Maxwell's rule and the Euler equation to obtain two proportionality conditions which relate the number of faces and the number of vertices and respectively the number of faces and the number of edges. Accordingly, Eq. (3) becomes:

$$E = 3V - 6 \ . \tag{4}$$

Now we substitute the previous equation into the Euler equation (for a simply connected polyhedron), finding the first condition which relates the number of faces and the number of vertices:

$$V = \frac{F}{2} + 2 \ . \tag{5}$$

Substituting once again the previous condition into the Euler equation we obtain the second condition which relates the number of faces with the number of vertices:

$$E = \frac{3}{2}F \ . \tag{6}$$

In our investigations the number of faces F corresponds to the number of carbon atoms (e.g. see Fig. 1). It has been proved that at least one spherical fullerene with X carbon atoms exists for all even X with $X \geq 20$ except for $X = 22$.

Each fullerene polyhedron has $V = 12$ vertices with five adjacent faces and so Eq. (5) implies:

$$V_6 = \frac{X}{2} - 10 \ , \tag{7}$$

where V_6 is the number of vertices with six adjacent faces/carbon atoms. Although $V_6 = 0$ in our case, Eq. (7) is of general validity [7] also for $V_6 \neq 0$.

From a chemical point of view, the interest centers on isolated-pentagon fullerenes, which can be constructed for $X = 60$ and for all even value of $X \geq 70$ (e.g. C60 having twelve pentagons and twenty hexagons).

3 MOLECULAR ARCHITECTURES

A fullerene can also be seen as a trivalent graph with hexagonal and pentagonal faces [8-10]. Fullerenes, and nanotubes in particular, can be obtained by rolling a sheet of graphite. Depending on how the sheet is rolled up, we have three kinds of nanotubes. The dash lines in Fig. 3 denote the main symmetry directions in the graphene sheet:

(n,0) zigzag, (n,n) armchair, (n,m) chiral
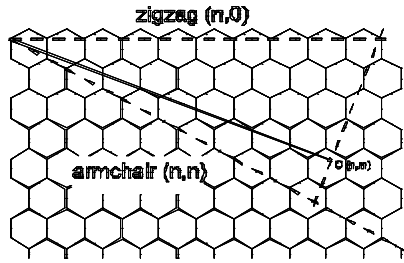
Fig. 3. Graphene sheet and nanotube chirality.

The special symmetry directions in the grapheme lattice are (n,0) and (n,n); they differ by an angle of 30°. The name armchair and zigzag refer to the pattern of carbon bonds along the circumference. The pair of indices (n,m) identifies the nanotube and each (n,m) pair corresponds to a specific set of chiral angle ϕ and diameter d :

$$\phi = \arccos\left(\sqrt{3}(n+m)\Big/\left(2\sqrt{n^2 + m^2 + nm}\right)\right), \tag{8}$$

$$d = \frac{\sqrt{3}a}{\pi}\sqrt{n^2 + m^2 + nm} \quad, \tag{9}$$

where a is the C-C bond length (normally a = 0.142 nm). The circumference and the diameters of nanotubes can be calculated by simply using geometrical properties:

$$\begin{aligned} C(n,n) &= \pi d_{n,n} = 3na \\ C(n,0) &= \pi d_{n,0} = \sqrt{3}na \end{aligned}. \tag{10}$$

Normally carbon nanotubes grow inside other nanotubes forming multi-walls; so it is worthwhile compare different diameters. If $n \leq m$

$$\frac{d_{n,n}}{d_{m,m}} = \frac{n}{m} , \; \frac{d_{n,0}}{d_{m,0}} = \frac{n}{m} , \; d_{n,0} = \frac{\sqrt{3}}{3}\frac{n}{m}d_{m,m} , \tag{11}$$

and the interlayer distance between the outer and the inner diameter is:

$$t_{(m,0)(n,n)} = \frac{1}{2}\left(1 - \frac{n}{m}\sqrt{3}\right)d_{m,0} = \frac{\sqrt{3}a}{2\pi}\left(m - n\sqrt{3}\right) , \tag{12a}$$

$$t_{(m,m)(n,n)} = \frac{1}{2}\left(1 - \frac{n}{m}\right)d_{m,m} = \frac{3a}{2\pi}\left(m - n\right) , \tag{12b}$$

$$t_{(m,0)(n,0)} = \frac{1}{2}\left(1 - \frac{n}{m}\right)d_{m,0} = \frac{\sqrt{3}a}{2\pi}\left(m - n\right) . \tag{12c}$$

From a chemical point of view when carbon atoms combine to form graphite, $sp2$ hybridization occurs [11]. In this process one s-orbital and two p-orbitals combine to form three hybrid $sp2$ orbitals at 120° to each other within a plane [12] as shown in Fig. 4. This in-plane bond is a strong covalent bond that binds the atoms in the plane.
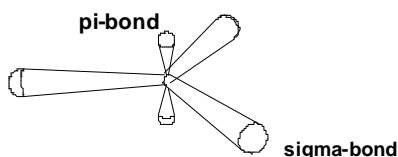
Fig. 4. A representation of the $sp2$ hybridization.

In deltahedra $(n,0)$ and (n,n) this in-plane bond interacts as cylindrical hinge with a rotational axis perpendicular to the $sp2$ orbital axis (Fig. 5). The nanotubes $(n,0)$ and (n,n) can be modelled by simply using a planar tripod, while chiral nanotubes (n,m) cannot be included in the family of deltahedra (Fig. 6).
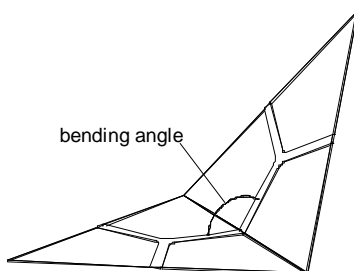

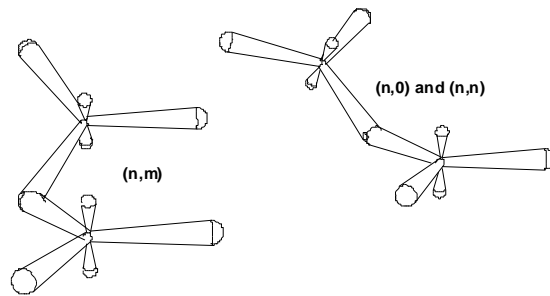Fig. 5. A planar model with bending angle in deltahedra.

Fig. 6. Orbital distorsion for (*n,m*) geometries.

What follows are eight figures (Figs. 7-14) with different models of fullerenes: zig-zag e armchair; we start from the smallest C(2,2) e C(3,0) which probably do not exist in nature as carbon molecules in fact at ends have vertices with three or four adjacent atoms; perhaps they could be boron molecules, element which presents *sp*2-hybridized atoms.

We will also show a model of nanotube C(3,3) which is considered by Iijima [13] the smallest fullerene existing in nature.

$$X = 8 + 8k$$
$$V = 10 + 4k \qquad k = 0,1,2.....n$$

X = number of elements
V = number of vertices
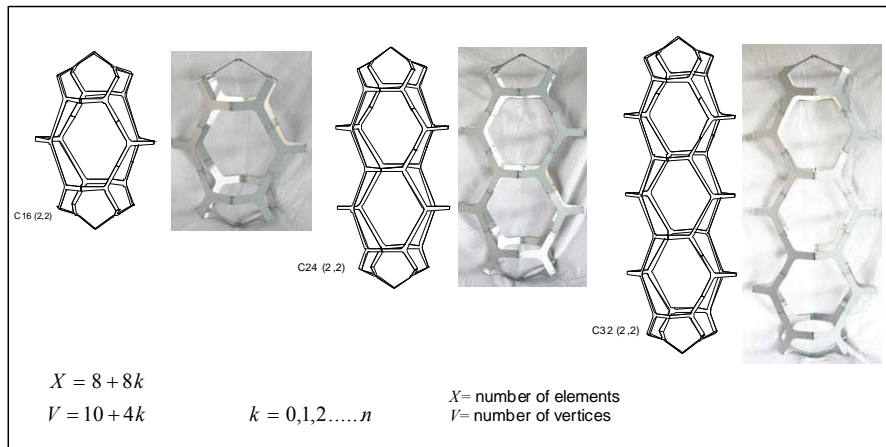
Fig. 7. Examples of nanotube with chiral index (2,2) and its practical realization.

Non-chiral nanotubes will be shaped by an aluminium tripod and cylindrical hinges at the ends, which make it possible to build objects on all planar faces. As for chiral nanotubes, tripods made of plastic will allow for arms distortion.
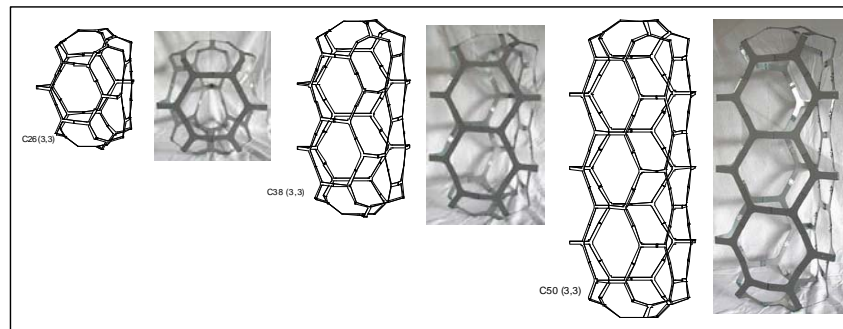
Fig. 8. Examples of nanotube with chiral index (3,3) and its practical realization.
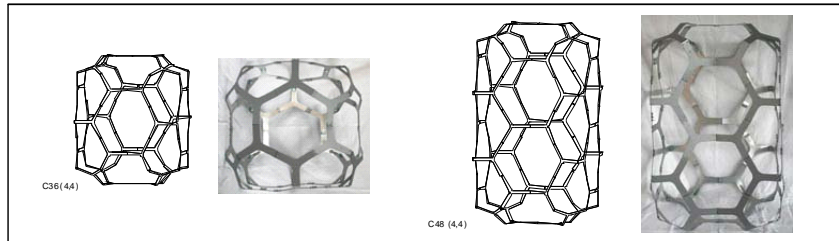
Fig. 9. Examples of nanotube with chiral index (4,4) and its practical realization.

Fig. 10. Examples of nanotube with chiral index (3,0) and its practical realization.
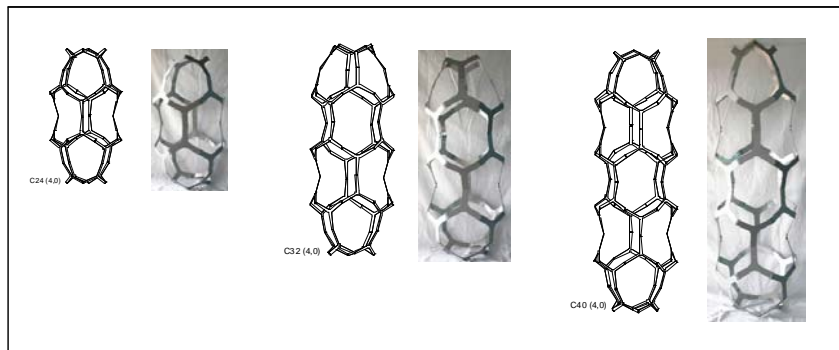

Fig. 11. Examples of nanotube with chiral index (4,0) and its practical realization.

Now we will show different geometrical forms of fullerene with 60 carbon atoms (Figs.15-19); all of these forms are characterized by twelve five-membered rings and twenty six-membered rings.
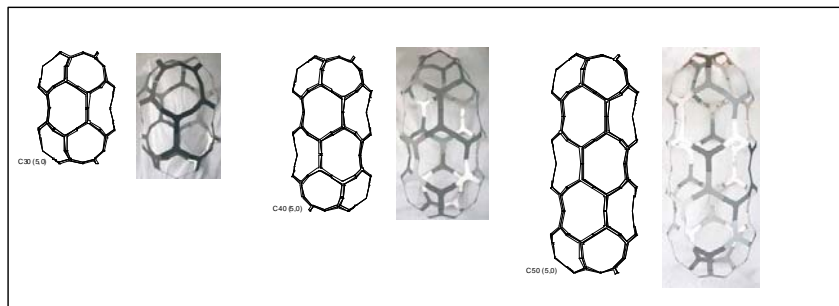

Fig. 12. Examples of nanotube with chiral index (5,0) and its practical realization.
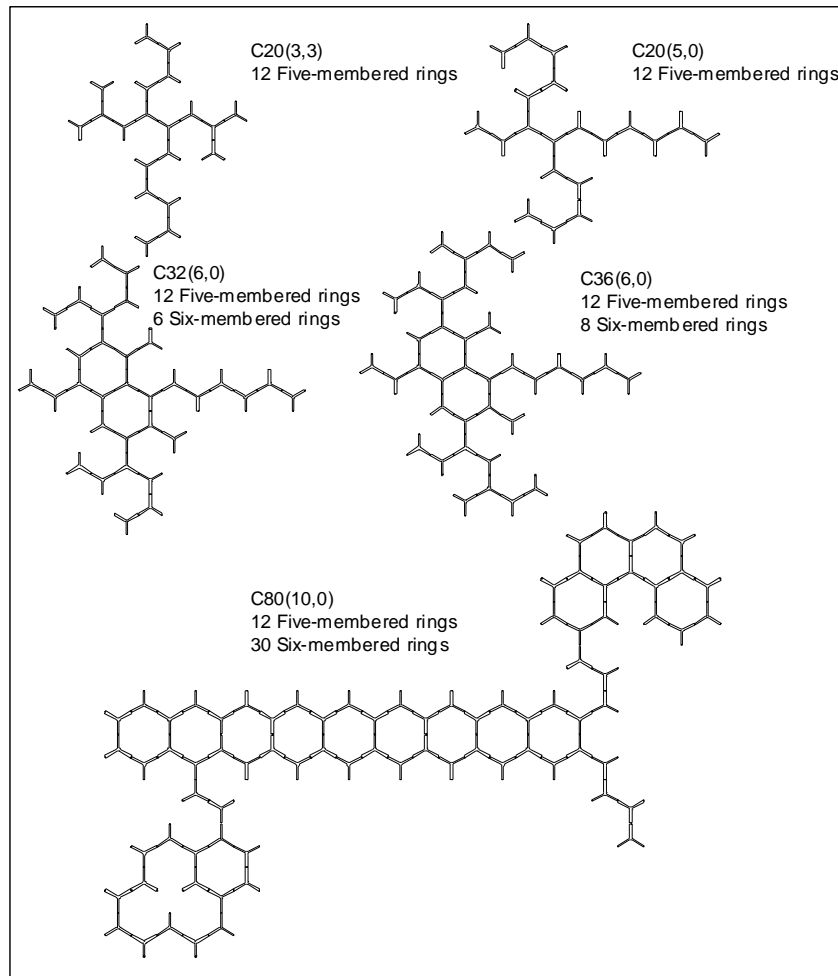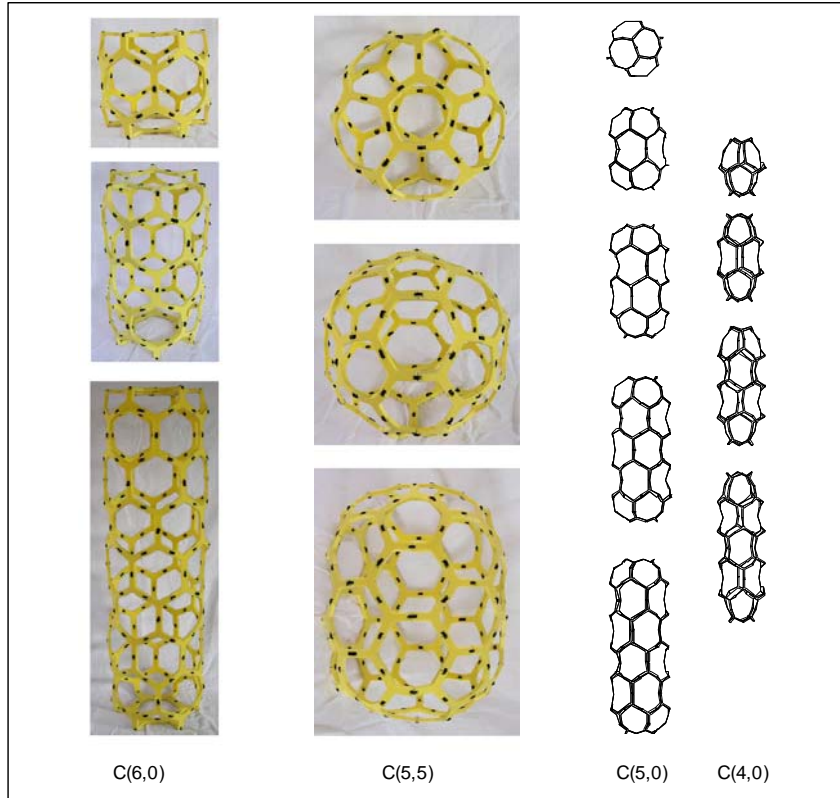
Fig. 13. Examples of planar development.

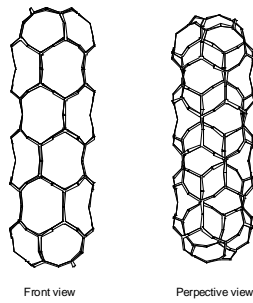Fig. 14. Examples of growing sequence.

Front view   Perpective view

Fig. 15. The C60 (5,0) structure.

Front view   Perspective view
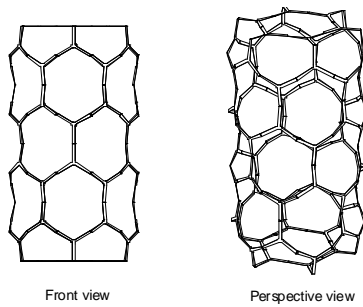
Fig. 16. The C60 (6,0) structure.

Front view   Perspective view
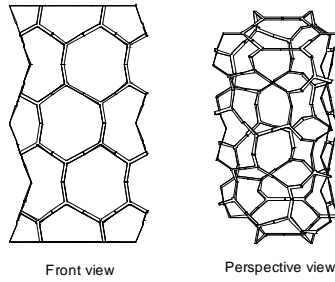
Fig. 17. The C60 (6,0) structure with different bending angles.

Front view   Perspective view

Fig. 18. The C60 (6,6) structure.

Front view   Perspective view
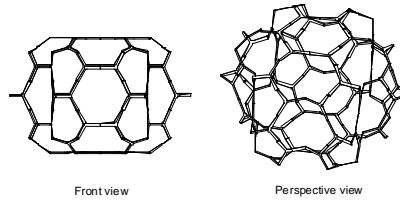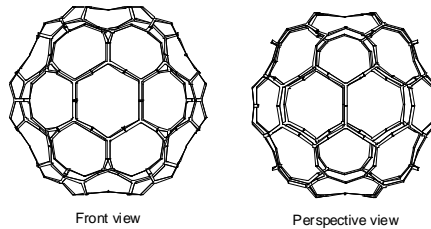
Fig. 19. The C60 (5,5) structure.

Fullerene C60 can be considered as particular case of the family of nanotubes with chiral index (5,5) and the calculated radius is quite interesting:

$$r_{5,5} = \frac{3}{2\pi} 5(0.142) = 0.340 \text{ nm} .$$ (13)

The value obtained is equal to the distance between successive planes in graphite. The only fullerene cage, in which all twelve pentagons are completely surrounded by hexagons, is fullerene with chiral index (5,5). We have found, realizing models of capped nanotubes C(n,n), that, increasing the value of the chiral number n the cross-section of the capped nanotube tends to become flat if we respect the rule of the twelve pentagons (Fig. 24 shows an example).

4 BIOLOGICAL ARCHITECTURES

Carbon, in nature, presents different macro-molecular forms (eg. diamond and graphite); it is the base of the organic chemistry, the pillar of every living being. We have found a possible analogy between snake scales and fish scales and nanotubes. The Fig. 20 shows a growing sequence in which the symmetry directions for a nanotube are highlighted.
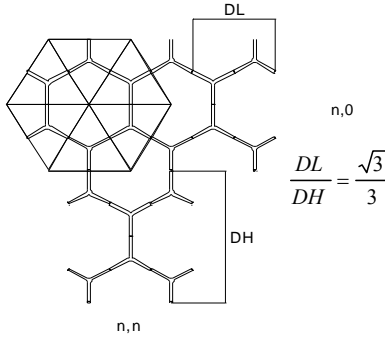

$$\frac{DL}{DH} = \frac{\sqrt{3}}{3}$$

Fig. 20. Example of growing sequence.

The direction (n,n) grows more rapidly than the direction $(n,0)$. A nanotube $C(n,0)$ is obtained by rolling a sheet of graphite along the symmetry direction $(n,0)$; Fig. 21 shows a nanotube $C(10,0)$, we observe an analogy between the snake in Fig. 22; we see that the scales are rolled along the direction $(n,0)$, while the length of the snake develop along the direction (n,n). Normally a snake presents a small diameter respect the total length and the nature seems to favour the $C(n,0)$ pattern and this is a consequence of the different growing factor between the two symmetry directions.

Figure 23 shows the flank of a fish, aquatic animals that are typically covered with scales and equipped with two sets of paired fins and several unpaired fins; in this case, the fish scales develop along the radial direction as a nanotube $C(n,n)$. Normally a fish presents a shape with a frontal section, not round but slightly flat at two extremities; on the contrary respect to a snake, where we observe a round cross-section and a total length predominant respect the diameter, in a fish this phenomenon is not so plain. Probably, this analogy between nanotubes, snake scales and fish scales is a particular case of approximation of a surface using discrete geometries (eg. Voronoi diagrams, Delaunay triangulation).
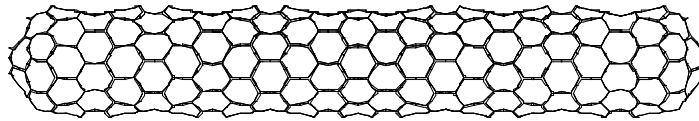

Fig. 21. The C (10,0) structure.
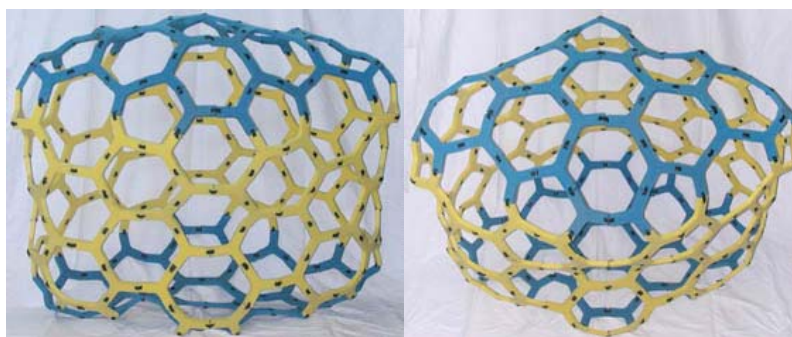
Fig. 22. Snake scales.

Fig. 23. Fish scales.

Fig. 24. Capped nanotube C(*n,n*) with a flat cross-section.

5 MACROSCOPIC MOLECULAR INSPIRED ARCHITECTURES

From an architectural point of view, it is interesting to face the problem of how to build a structure taking advantages of the same indices used to characterize the nanotubes. We define a box (Figs. 25, 26) with three cardinal dimensions A,B,C in which we want to insert a structure mimicking a nanotube C(n,0) or C(n,n). Assume C to be along the longitudinal axis, that is the nanotube length. Searching the radius of the circle having a section of base A and height B gives geometrically the radius R of the nanotube-like macrostructure as:

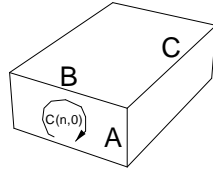$$R = \frac{B^2 + A^2/4}{2B} \,. \tag{14}$$
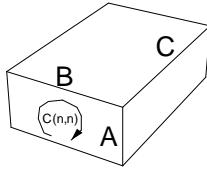

Fig. 25. The C(n,0) box.

Fig. 26 The C(n,n) box.

Accordingly, from Eq. (9), setting $2R = d$ and $m = n$ or $m = 0$ we deduce the proper chiral number n for nanotube-like macrostructures C(n,0) or C(n,n):

$$n = \frac{\pi}{\left(\sqrt{3}\right)^\alpha} \left(\frac{B}{a} + \frac{A^2}{4Ba} \right), \tag{15}$$

where $\alpha = 1$ for C(n,0) or $\alpha = 2$ for C(n,n) and a is the length of the macroscopic bond. The number of the required tripod elements is predicted by our analogy to be:

$$X = \frac{4nC}{(\sqrt{3})^\beta a} \,, \tag{16}$$

where $\beta = 1$ for C(n,n) or $\beta = 2$ for C(n,0). With Eqs. [14]-[16] we can design macrostructures mimicking carbon nanotube architectures.
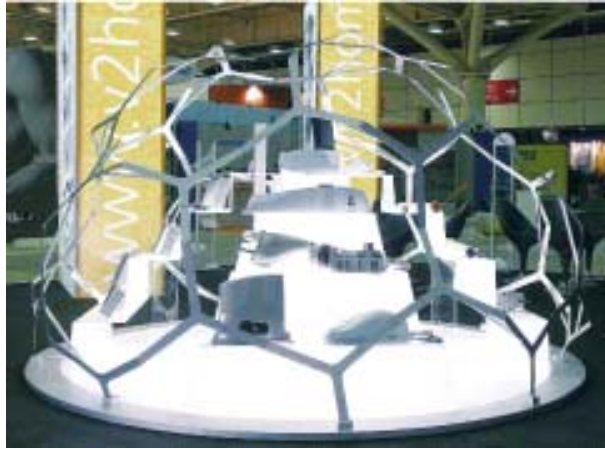
Fig. 27. V2 stand exhibition fair Bologna (Courtesy G.T.C.A. Srl Grid Structures).

Now let us consider a dome for exhibition purposes as a way to continue our analogy between molecular structures and geometrical and architectural structures (Fig. 27). The structure reported in Fig. 27 is made of 30 tripod-like aluminium elements connected by cylindrical hinges; sticks in each of the junctures of the faces made by five elements of the fullerene make the structure stable.

The dome is half–fullerene and we consider fullerene as a (5,5) fullerene with $a = 0.6$ m (macrosco5pic bond).

$$d_{5,5} = \frac{3}{\pi} 5(0,6) = 2.9 \text{ m.} \qquad (17)$$

A roof-like structure for a tennis court provides another example. The starting point is a nanotube semi-cylinder C(10,10) Fig. 28; the two-story geometric structure guarantees the necessary resistance (Fig. 29).

$$d_{10,10} = \frac{30}{\pi} a = 19 \text{ m} , \qquad (18)$$

$$l_{9,0} = \sqrt{3} na = 31,2 \text{ m.} \qquad (19)$$

The tripod-like element gets bigger and is developed on two links, one equilateral triangle-like module for the external link and one hexagon-like module for the internal link. The whole structure is made of 180 of such units (Fig. 30). The external link resembles the way in which Chinese peasants weave their baskets, also known as Kagomé grid [14-16].
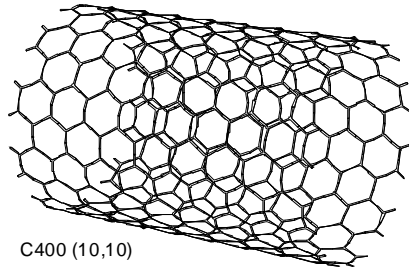
C400 (10,10)

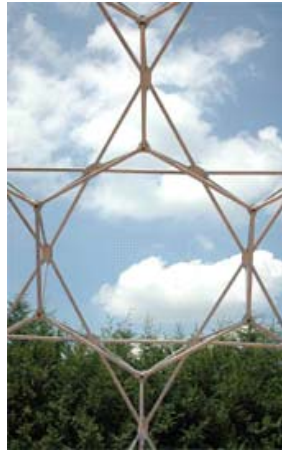Fig. 28. The C400 (10,10) reference nanotube.

Fig. 29. A double layer geometry: practical realization.

Fig. 30. Tennis court cover Racconigi (Courtesy G.T.C.A. Srl Grid Structures).

Another example is provided by an educational game (Fig. 31). The element is injection-moulded; the material used is thermoplastics resin (acetalic); the element consists of a body of

a planar tripod, with three equidistant arms whose free ends are arranged to be angularly deviated from a same side relative to the general plane of the tripod body to achive their union with the free ends of the arms of similar tripod bodies.

The hooking is realized by means of snap-fit (Fig. 32); the outcome is the structural equivalent of a joint. This element is helpful as it highlights the deformation underway in a chiral nanotube (*n,m*), which confirms what has been said earlier (Fig. 33).
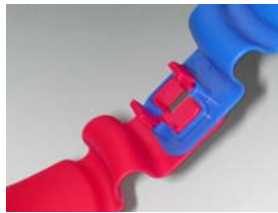

Fig. 31. A piece of the educational game.

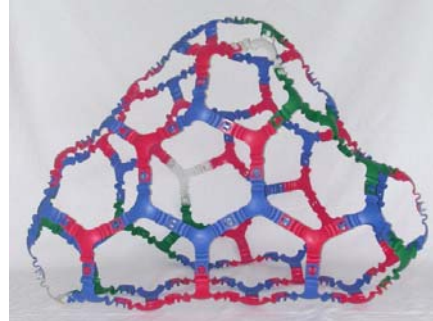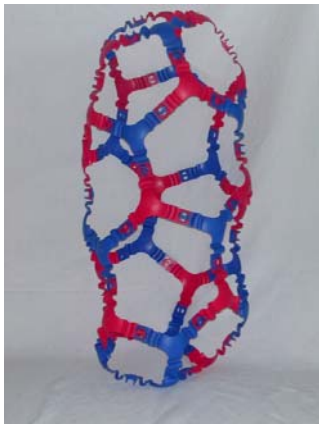Fig. 32. The snap-fit of the educational game.

Fig. 33. Models of chiral nanotubes C(*n,m*): practical realizations.

6 CONCLUSIONS

We have shown that there is a close analogy between some kinds of deltahedra and molecular structures which are typical in fullerenes. By introducing an architectural analogy between a tripod-like planar element allows for the realization of nanotubes models C(*n,n*) and C(*n,0*) at the macroscopic level. From an architectural point of view, we have showed new macro-structures as well as a geometrical toy model. The use of this element to build tri-dimensional grids, in which elements are not simply connected with each other, is a further step in this direction.

Acknowledgments

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