

## WHAT DIAMOND SPEAKS ABOUT?

© V.N. Poljansky & I.V. Poljansky, 2005

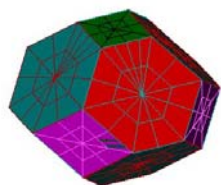
The idea of this research has arisen after we have found out a glaring contradiction between actual density of carbon in diamond and graphite, and theoretical density of carbon in fullerene C60.

According to the official paradigm of quantum chemistry, fullerene C60 contains 60 atoms of carbon. Its external diameter is equal 0.7nm, internal – 0.44nm. The surface of the fullerene is made of twenty hexagons and twelve pentagons. Having calculated the mass of sixty atoms of carbon and volume of a spherical layer of the fullerene C60, we can find out density of carbon in this design. It is equal 8857 kg/m<sup>3</sup>, that 2.5 times is more, than the density of diamond, and 4 times is more, than density of graphite.

According to our polytronic model, this fullerene contains only 24 atoms of carbon. In this case, the density of carbon in fullerene is equal 3543 kg/m<sup>3</sup>, i.e. it differs from density of diamond for 0.9 percent.

To confirm validity of polytronic model, we have made exact calculations and graphic constructions of crystal lattices of diamond and graphite.

In fig.1 the shape of atom of carbon is shown. The atom has the shape of the truncated octahedron with fourteen sides – 8 hexagonal sides (4 red and 4 blue), 4 rhombic sides (lilac color) and 2 square sides (green color).



**Fig. 1**  
**Polytronic model of atom of carbon**

The hexagons conditionally designate polytrons. Red hexagons are radial polytrons; blue hexagons – axial polytrons. The diameter of polytrons is equal  $D=0.1676\text{nm}$ . The long diagonal of rhombus is equal  $D$ , the short diagonal is equal  $D/\sqrt{2}=0.1186\text{nm}$ . The edge of green square is equal 0.0868nm. The dihedral angle at the top of octahedron is equal 90°.

From atoms of carbon it is possible to combine two types of cluster.

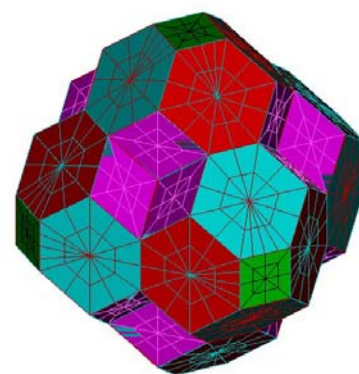
In fig.2 a cluster C6, which consists of six atoms is shown; in fig.3 a cluster C12 of twelve atoms is shown. In the center of cluster C6 the cavity, as cubic cell (fig.4a), is located. The cavity in the center of cluster

C12 represents rhombohedral dodecahedron (fig. 4b).

The crystal of diamond consists of clusters C6, which densely adjoin one to other by planes of two hexagons. In crystal of diamond a distance between cubic cavities is equal 0.324nm, a distance between rhombohedral cavities is equal 0.458nm, a distance between cubic and rhombohedral cavities is equal 0.281nm.

External surfaces of clusters C6 and C12 can adsorb atoms and molecules of carbon. At that, around of clusters the shells of atoms are formed, which have received the name of fullerenes.

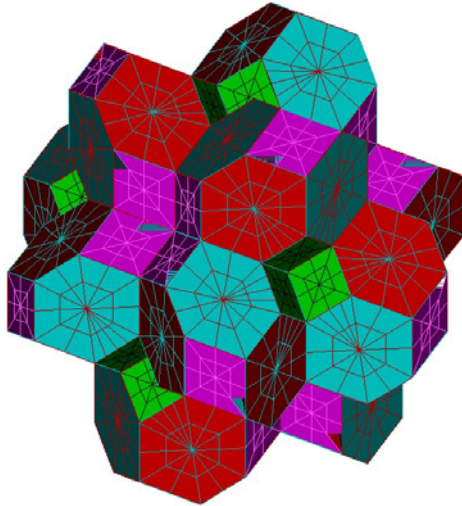
Cluster C6 has twelve directions for growth of shells. Each direction is a perpendicular from a plane, which consist of two hexagons. Hence, the first shell has two atoms in each direction of growth, and the first fullerene consist of twelve pairs of atoms of carbon, i.e. it is fullerene C24. The minimal internal diameter of fullerene C24 is equal 0.458nm. Diameter on the centers of pairs atoms in the first shell is equal 0.686nm, diameter on the centers of atoms in the first shell is equal 0.724nm, average diameter of shell is equal 0.705nm. The second layer of atoms is adsorbed on atoms of the first shell. The second shell, as well as the first, consists of 24 atoms, but pairs atoms in the second shell are located perpendicularly relative to pairs atoms in the first shell. Thus, the two-layer fullerene consist of 48 atoms, i.e. it is fullerene C48. Diameter of an external shell of fullerene C48 on the centers of pairs atoms is equal 0.916nm, diameter on the centers of atoms is equal 0.972nm, average diameter of the second shell is equal 0.944nm.



**Fig. 2**  
**Carbon cluster C6**

The third layer of atoms (also 12 pairs atoms) is adsorbed on atoms of the second shell, but pairs atoms in the third shell are located perpendicularly relative to pairs atoms in the second shell. Thus, the three-layer fulleren consist of 72 atoms, i.e. it is fulleren C72. Diameter of an external shell of fulleren C72 on the centers of pairs atoms is equal 1.145nm, diameter on the centers of atoms is equal 1.168nm, average diameter of the third shell is equal 1.156nm.

Fulleren C72 is the strongest and stable in comparison with fullerenes C48 and C24.



**Fig. 3**  
**Carbon cluster C12**

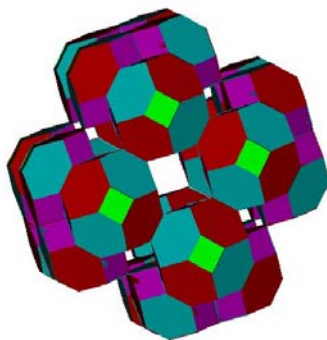
On a surface of cluster C12 six centers of rhombohedral cavities and eight centers of cubic cavities are located. Hence, cluster C12 has favorable opportunities for growth of the first shell. The first shell has four atoms around of each rhombohedral center or three atoms around of each cubic center. Hence, the first shell around of cluster C12 has 24 atoms, i.e. as much, as in the first shell around of cluster C6. But "three" of atoms in this shell are directed inside of a fulleren. Therefore, the energy status of this shell is more favourable, than energy status of the first shell around of cluster C6. Together with cluster C12, the first shell forms fulleren C36. In the center of fulleren C36 the rhombohedral cavity by diameter 0.167nm is located.

Diameter of an external shell of fulleren C36 on the centers of atoms is

equal 0.724nm. In fig. 5 the external shell of this fulleren is shown. We have designated this composition from 24 atoms, as fulleren C(36–C12)R. Here, by sign "-" the minus is designated; by letter R – type of the center.

The geometrical shape of a fulleren does not allow speaking concerning exact values of external and internal diameters.

External diameter of fulleren C(36–C12)R is approximately equal 1nm; its internal diameter is approximately equal 0.47nm.



**Fig. 5**  
**Fulleren C(36–C12)R**

Through the center of cluster C12 it is possible to build conditionally six planes of sections through hexamerous rings. At that, we shall find out, that clusters C12 can be of two types. Clusters of the first type have the left rings (see fig.6a), clusters of the second type have the right rings (see fig.6b).

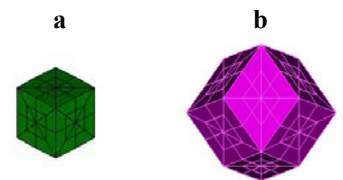
Besides, we can conditionally dismember cluster C12 in four of "three" of atoms. At that, we shall find out, that the left cluster C12 will consist only of "the left three" atoms, whereas the right cluster will consist only of "the right three".

Accordingly, cluster C6 will consist of one "left three" and one "right three".

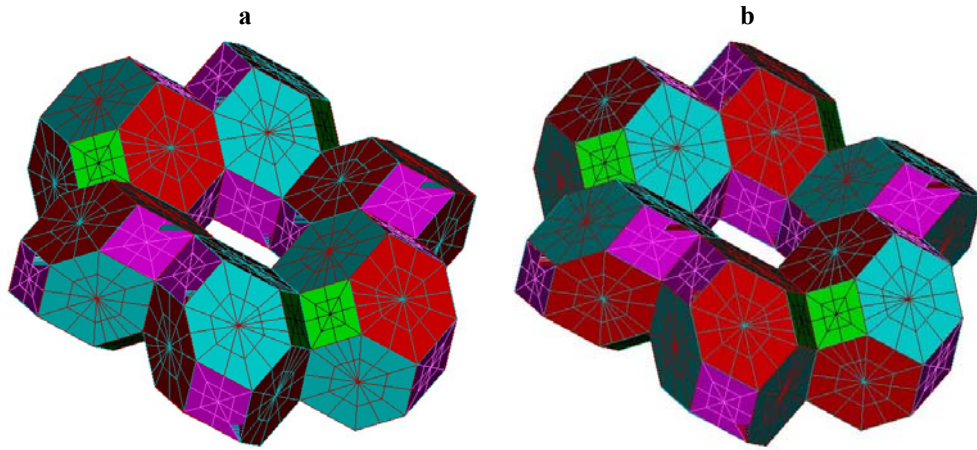
The properties of clusters C6 and C12, that are described above, determine the law for adsorption of external shells around of clusters. So, for example, the first shell around of left cluster C12 consist of eight "right three".

The crystal structure of graphite is formed of hexamerous rings and clusters C6. Hexamerous rings form flat grids. The grid of the left rings is shown in fig.7.

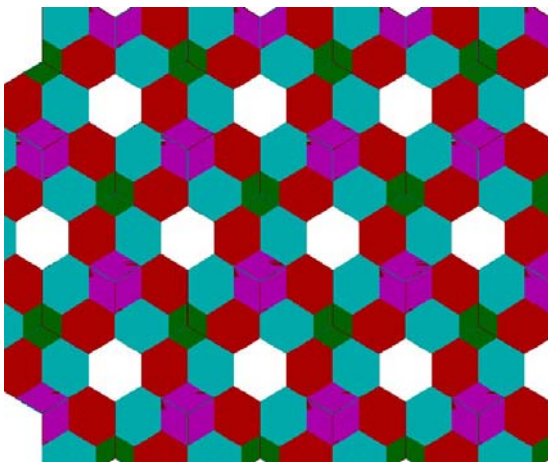
Graphite consists of parallel grids, between which clusters C6 are located. This structure is similar to the ball-bearing. Therefore, graphite has the good antifrictional property along grids. But across grids, graphite is very fragile.



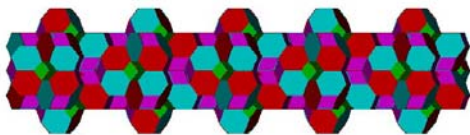
**Fig. 4**  
**a) The cubic center of a cluster C6**  
**b) The rhombohedral center of a cluster C12**



**Fig. 6**  
a) left ring; b) right ring



**Fig. 7**  
Carbon grid of left rings



**Fig. 8**  
Carbon nanotube of five clusters C12

Therefore, the statement by the official paradigm about that, the nanotubes represent convoluted, as cylinder or as roll, grids is the gross blunder. We suppose, that nanotubes represent “accrete” clusters and fullerenes.

One of such designs is shown in fig.8. This nanotube consist of three left and two right clusters C12. The nanotube has no a transparent aperture. Inside the tube the row of alternating rhombohedral cavities is located.

It is conditionally possible to accept, that nanotube of clusters C12 has hexahedral shape.

According to our calculations, the thinnest nanotube will consist of incomplete clusters C6.

Each unit in this nanotube will consist of five atoms. The shape of nanotube represents a roundish octagonal rod. Average value of external diameter of rod is equal 0.5nm.

It is obvious, that nanotubes of big “accrete” fullerenes also have articulate (or wavy) surface and more leveled transitions between units.

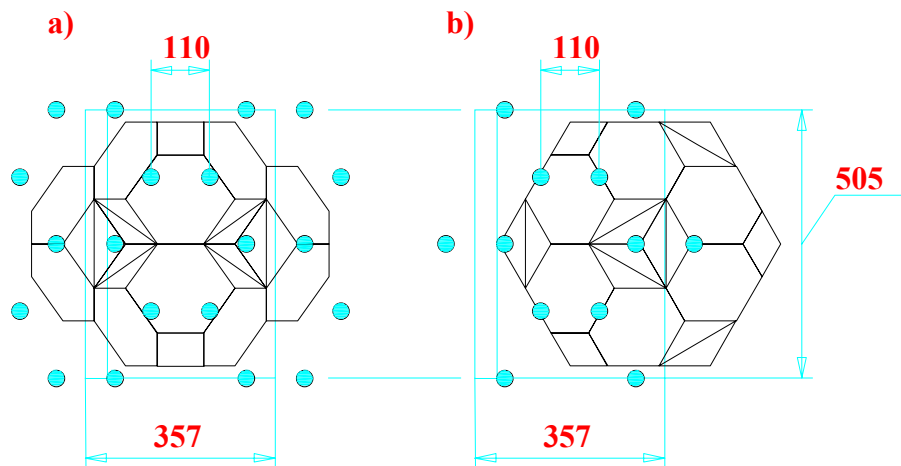
The model, offered by us, allows calculating the shape and the sizes of fullerenes and nanotubes more precisely and, hence, more precisely to predict their physical and chemical properties.

### **Postscript**

For experimental checkout of the foregoing stereographic constructions we have used of the electronic microphoto of a surface of diamond in a plane [110]. This popular microphoto has been made in the middle of the XX-th century and it can be found in many directories.

We have executed two projections of the specified microphoto on carbon cluster C6 (fig. 2), corresponding to hexagonal crystal structure of diamond and have received the mentioned below picture (see fig. 9).





**Fig. 9. Image of carbon cluster C6 at frontal view on a hexagonal cell (the left drawing) and at the sight under angle 35.26° (the right drawing). The sizes are given in picometers. Blue stains ostensibly indicate an arrangement of atoms on surfaces of a crystal of carbon.**

As it is seen from fig. 9b, “electronic stains” of microphotos are located on edges of hexangular cells of cluster, i.e. in those places where there are located points of connection between the nearby atoms and radiating assemblies of polytrons.

As a result of our research there were quite reasonable two questions:

1) What Academy of Sciences has counted in fullerene C60 sixty atoms of carbon?



2) Who in first half of XX-th century has passed in an official paradigm by Rutherford's unchecked statement, that its alpha particles got to the nucleus thought up by him, which are in the centres of atoms?

After all it was absolutely obviously and in the XX-th century beginning, that any electrically charged particle flying with the high speed, is a power probe. Therefore, this probe, first of all, should "feels" points of the maximum power connection between atoms, but only not mythical nucleus of atoms.

~ ~ ~ ~ ~

The summary. *Fundamental errors in the physics of fullerenes and in the physics of atom are shown.*