Morphology Changes and Defects in Carbon Nanoparticles Due to Different Atom Arrangements

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ABSTRACT

Motivation: Pentagon and heptagon fullerene carbon nanostructures (CNT) have potentials in superlight weight industries. CNT have structural defects caused by irregular atom arrangement during CNT growth. For better use, it needs modifications to remove defects. To accomplish it, investigations were made to identify bad atom arrangement. Findings: Present study highlighted the following: 1. The arrangement of carbon atoms in CNT rings was complex and different from common 6 carbon atom ring in nature; 2.Structures with incorporated n-gons are a new kind of nanostructure composed of parts equal in atom arrangement joined with suitable carbon connection bonds; 3.Still a lot of bio-industrial and superlight-weight interest in these CNT structures is not focused because of n-gons structural properties are unknown in the entire CNT complex; 4. The carbon atom arrangement in n-gons may answer the troubleshooting the defects of lightweight CNT complexes as elements in nanoscale devices and composite materials; 5.The present nanotechnology development allows the complicated CNT nanostructures with limited known chemical properties in experimental conditions by using self-assemble processes and atom-by-atom manipulation in CNT; 6. The industrial demand is increasing for more specific superlight weight CNT nanocomposites with atomic properties suited to environmental climatic resistance with utrastrength in more complicated aero-industrial applications. Conclusion: To meet these industrial applications, the arrangement of n-gons in CNT structures become complicated with new applications tailoring with their modified arrangement in CNT structures. It also provides more functionality necessary through incorporation of different n-gons and their combinations. It also inspired the continuous and further study of the n-gon role, with the exception of pentagons and heptagons, on carbon nanoparticle properties.

Key words: CNT, nanomaterials, polygon

1 INTRODUCTION

Carbon materials are in the most stable energetic situation if their atoms are connected via sp3 bonds and build 6 atom rings (n-gons with n=6), which, on their side, construct a honeycomb-like network.

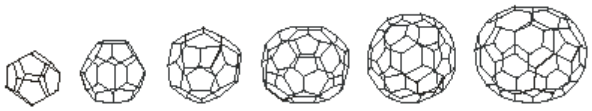

Fig 1:A general sketch shows different carbon nanotubes.

2 PENTAGON-HEPTAGON FULLERENES

Most favored emergence of n-gons with n = 5 and 7, explains honeycomb structure of the observed carbon nanoparticles. The simultaneous emerged 5/7 defects such as pentaheptite, defects oppositely situated in the nanoparticle structure and the repetitive pair and carbon network deformation. The rings of *n* atoms (*n*-gon), for *n* = 1 up to infinity, and the changes in the network due to an *n*-gonal defect. Fig. 2 illustrates the honeycomb network that corresponds to the *n*-gons, when *n* = 1, 2, 3, 4 and 5. The bird's-eye view of transformed network due to an *n*-gonal defect is shown in Fig. 2b for *n* = 3, 4 and 5.

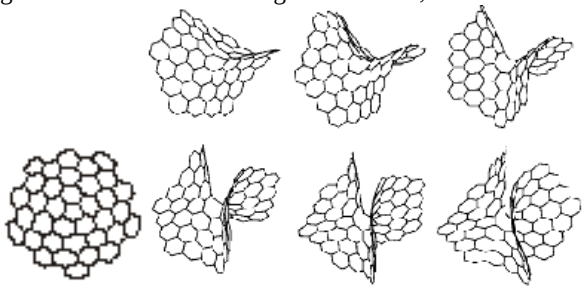

Fig 2: Honeycomb (left panel) and n-gonal defects of CNT

The rings of *n* atoms (*n*-gon), for *n* = 1 up to infinity, and the changes in the network due to an *n*-gonal defect, are widely discussed and explained in [47]. Fig. 2 illustrates the honeycomb network that corresponds to the *n*-gons, when *n* = 1, 2, 3, 4 and 5. The bird's-eye view of transformed network due to an *n*-gonal defect is shown in Fig. 2b for *n* = 3, 4 and 5. CNT can have defects similar to graphene (incorporation of carbon rings with $n \neq 6$). Defects change nanotube geometry, e.g., their diameter and chirality and through that their electronic properties without introducing any impurities. It gives the possible electronic properties via defect changing. Defect arrangement is stable in time and due to that electronic properties will stay constant for the whole time of tube existence. This is illustrated in Fig. 3 for 3 orientations (Fig. 3a) of the tube axe to the carbon-carbon bonds. The nanotubes will be (6,0), (6,2) and (6,6) and will have diverse diameters (see Fig. 3b,c). Their hexagons are arranged in a different way according to the nanotube axe

(Fig. 3b). Those 3 kind of CNT are known as zigzag (when n = 0), chiral (different from its mirror image and m ≠ n), and armchair (when m = n). That means that each possible pair of coordinates (m,n) corresponds to a nanotube which will have unlike orientation as compared to all the others and, hence, of different diameter.

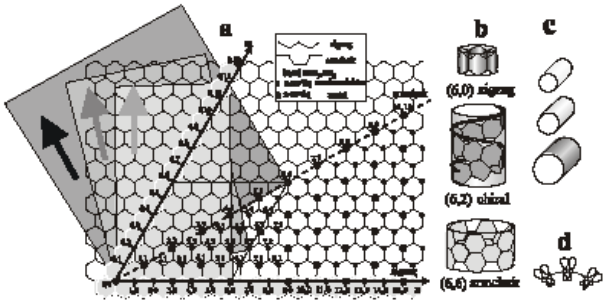

Fig 3: A coordinate system used for explaining carbon network and carbon structure properties. Three type of CNT (zigzag, armchair and chiral) are exhibited with their maps (Fig. 3a), their ring arrangement in accordance with tube axis (Fig. 3b), tube diameter (Fig. 3c) and a sketch of the electron orbital deformations by some bending (Fig. 3d).

- The pentagon and the heptagon are the frequently arising defects and can margin single or simultaneously in the nanotube structure. The single pentagon makes the circumference to decrease as the axis is extended behind the defect. On the contrary, the heptagon causes increasing of the tube circumference and the diameter. Merging of an isolated pentagon in the nanotube and transformation of the nanotube to a cone-like structure through that is illustrated in Fig. 4a. The tube is divided in two through the pentagon and the maps of the both parts are exposed right hands and left hands at the cut line DF of the pentagon. The exposition is over the carbon honeycomb to show how such a structure can be obtained via shearing the marked area and joining the line AB with A1B1 and CD with C1D1. In the case of the heptagon in Fig. 4b that is made analogically.

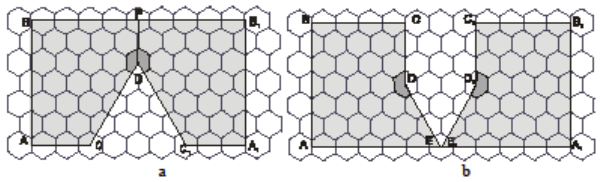

Fig 4: (a) a map of CNT with a pentagonal defect and (b) a map of CNT with a heptagonal defect.

- On the contrary, the defects caused by an isolated pentagon and a heptagon perturb the electronic properties of the hexagonal network significantly. If the symmetry axis of the aniline structure pair is nonparallel to the tube axis it changes chirality of a nanotube by one unit as shown in Fig 5. The heptagon splits the rows and as a result after the defect merging the row number 5 will be connected to number 4b instead to 5a after the map rolling in a nanotube. The pentagons arise frequently in pair with heptagons and they are responsible for the most of changes in the nanotube structures. The diameter extension becomes significant if the pentagon and the heptagon in the pair are separated by hexagons because each hexagon added between the pentagon and heptagon changes the nanotube circumstance by one unit as shown in Fig 4b. These pairs also rule the electronic behavior around the Fermi level. The pentagon and the heptagon in the pair can be isolated one to other or to have one joined edge as in the aniline structure. The effect of the 5/7 pair on the growing structure depends on its place and orientation to the network direction. When the pentagon is attached to a heptagon, the pair creates only a topological change, but no net disclination, which may be treated as a single local defect. The defect can be only a small local deformation in the width of the nanotube or a small change in the helicity, depending on its orientation in the hexagonal network.

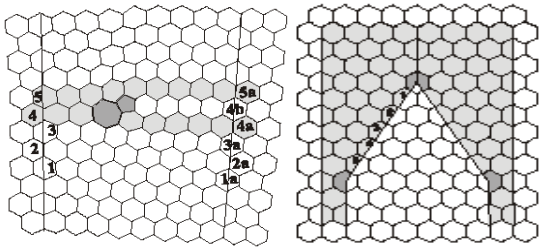

Fig 5: (left panel) A change of tube chirality by 5/7 defect nonparallel to tube axis. (Right panel) A change of tube circumference as a result of pentagon heptagon separation via 5 hexagons.

- The 5/7 pairs can be more than one in a junction zone. The pair can show different arrangements X-shape, T-shape, Y-shape, zig-zag, arm chair, double- and triple-strand and super coiled supercell e_x and e_y (determined in the honeycomb), L and M, and the vectors a and b defining nanoassemblies. In such case, polygonal defects other than pentagons and heptagons may play certain roles. The presence of up to 3 pairs in zigzag nanotubes in different configurations show several defects on the electronic properties of the system. The nanotube systems are (12,0); (11,0); (10,0) and (9,0). Those are selected because their electronic properties are expected to differ radically (the junction (12,0)-(9,0) is expected to be a metallic one, the two others are prototypes of a metal-semiconductor junction).

- A new class of layered carbon material, consisting of ordered arrangements of pentagons, hexagons, and heptagons is known as Haeckelites. They can be rectangular, hexagonal or oblique, surrounded by six-membered rings. They are more stable than C60 and can thus be regarded as energetically viable. All these structures are predicted to be metallic, exhibiting a high density of states at the Fermi energy, and to possess high stiffness. H5,6,7 and R5,7 haeckelites are predicted to be flat, while O5,6,7 is corrugated. H5,6,7 is found to be the most stable structure, possessing an energy of 0.304 eV per atom. All

Haeckelite nanotubes are metallic, independently of chirality and diameter.

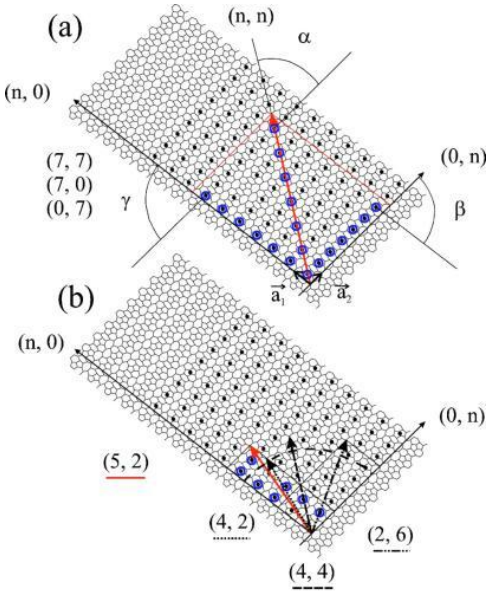

Fig 6 shows regular tiling of the plane with hexagons and azulene units in proportion 3:2.

- For illustration,'unit cell' is defined by the primitive vectors aW1 and aW2. The bonds shared by two pentagons have been highlighted by dots. In Fig 6(a), a 7x7 cell illustrates the wrapping vectors (7,0), (0,7), and (7,7) along the special directions (n,0), (0,n), and (n,n). The pentagons are encircled and rows are indicated by the thin solid lines defining the angles α, β, and γ. These rows can generate helical patterns along the structure. In Fig 6(b), the wrapping vectors (4,2), (5,2), (4,4), and (2,6) are highlighted by encircling. In the unit cell (2,6), all stressors are symmetrically placed around the wrapping vector. The dashed-line circle corresponds to a critical nanotube radius of 0.45 nm above which some stressors can dip inward toward the structure.

- The buckyballs have two aligned double bonds, each one in the center of a 5/6/6/5 pyracylene. This orientation conveniently permits standard polymerization by C60-pairs coalesce into the sections of (5,5) tubes either numbers 0 and 1 are the separate and the dimerized buckyballs.

- The nanopeapods are a family of carbon nanostructures where the condition for buckyballs coalescence is found to play significant role. Nanopeapods consist of an array of fullerene molecules (inner peas) and a single-wall carbon nanotube (SWCNT) (an outer pod), and all components are separated from the others by the van der Waals distance. Stable defects incorporated already in the nanostructures can also influence the growth of multi wall carbon nanotubes (MWCNT) growth. Each layer acts as a template for the sequent. During the simultaneous growth the atoms which achieve opened layer ends are under the influence on the attracting forces from the neighbor layers and at suitable conditions can connect both layers, seamed them in one closed surface as shown in Fig 7. Fullerenes start to coalesce at 800ºC and complete transformation to a single-wall nanotube at 1200ºC. fullerenes start to coalesce at 800ºC and complete transformation to a single-wall nanotube at 1200ºC.

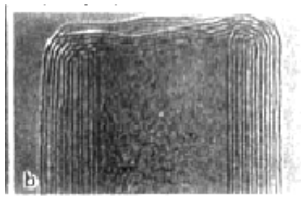

Fig 7: Sketch of nanotubes is shown with shells seamed one to other at the end of the tube.

- The defects and the electronic states initiated through that depend on tube type and size. The change in the rings of nanotubes (with different carbon network orientation to their axis) by adsorption of carbon dimers is shown in Fig 8.

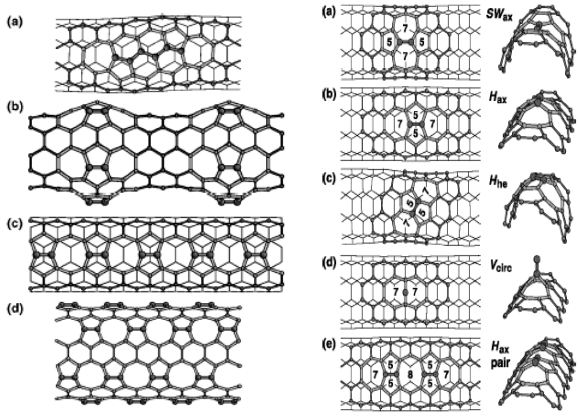

Fig 8(on left) Structure of multiple C-2 adsorbates.
Fig on right) Bonding structure of carbon dimer defects on a sample armchair (5,5) nanotube.

3 LIMITATIONS

Pentagons and heptagons emerged in the carbon nanostructures (CNT) as nano scale defects caused by irregular atom arrangement during growth. From this point of view, the induced investigations were attempted to pinpoint the reasons for bad atom arrangement and how those can be managed. From another point of view, the arrangement of carbon atoms in rings different from 6 carbon atom ring is also normal in nature, and in this case the structures with incorporated *n*-gons are to be treated as a new kind of nanostructure composed of parts equal in atom arrangement joined with suitable carbon connection bonds. There still remains lot of interest in those CNT structures, not focused before more on *n*-gons but on their structural properties of the entire CNT complex. Regardless of how

the differences in carbon atom arrangement are studied or viewed, they still remain an interesting and a very important subject for study because of the utility of nanoparticles as elements in nanoscale devices and composite materials.

4 FUTURE PROSPECTS

The continuous progress in nano-science and nanotechnology stimulates the creation of nanostructures with new properties and functions. The level of nanotechnology development at the present moment allows complicated nanostructures constructed and their planned properties to be realized via suitable conditions by using self-assemble processes and atom-by-atom manipulation. The more increasing demand for specific CNT particle properties increased the more complicated applications. As the structures become complicated their more frequent applications tailoring with their structures and functions are necessary through incorporation of different *n*-gons and their combinations. It inspired the continuous and further study of the *n*-gon role, with the exception of pentagons and heptagons, on carbon nanoparticle properties.

5 REFERENCES

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[i] http://www.scribd.com/doc/18663985/Nano-Materials-Lectures/ pages 352-85.