VERSATILITY OF SUPERCARBON NANOSTRUCTURES

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ABSTRACT

Carbon nanostructures, namely, fullerenes play an important role among many nanoscale materials investigated. The carbon nanotubes are the linear fullerenes which can have aspect ratios as large as 10^3 to 10^5. It has been observed that the nanotubes when self assembled usually form ‘Y’, ‘X’ or ‘T’ like stable junctions and can be manipulated to make orderly structures by exposing to electronic beams at high temperature during synthesis. When single walled carbon nanotubes (SWCNTs) are arranged to form a higher order structure, it is called a supercarbon nanostructure. The supercarbon nanostructures can be arranged in a variety of geometries with different junctions of SWCNTs and also the constituent SWCNTs can be varied in diameter, chirality and length. Therefore the supercarbon nanostructures are expected to have more versatile range of properties than the SWCNTs and graphenes.
This study focuses on physics of different geometries of supergraphenes, super nanotubes and supercubes which can be formed using different kinds of SWCNTs and their expected differences in mechanical, physical and electrical properties.

Key words: Single walled carbon nanotubes, Y junctions, supercarbon nanostructures

1. INTRODUCTION

Even though first introduced by R. P. Feynman in 1959, the nanodiscoveries and capabilities of building materials at atomic or molecular scale was slow until the emergence of Scanning Tunneling Microscope and other sophisticated measuring instruments in 1980’s.

Synthesizing super nanostructures from single walled carbon nanotubes (SWCNTs) as building blocks and predicting their mechanical, electrical and thermal properties have become an immense challenge to the researchers in the field of nanotechnology. Super nanostructures made up from SWCNTs are expected to have outstandingly different characteristics to the constituent SWCNTs, which will be used in future nano electromechanical systems (NEMS) [1].

SWCNTs can be manipulated to have junctions by introducing defects such as pentagons and heptagons in to usual hexagonal array of carbon atoms in super carbon nanostructures. Different types of junctions are being produced while forming super nanostructures [2]. By changing the manufacturing process it is anticipated to get orderly Y, X and T junctions. It is predicted that super nanostructures of different junctions have unique electrical, mechanical, thermal, optical and magnetic properties. At the same time the properties of the constituent SWCNT i.e. the chirality (n), diameter (d) and length (L_o) also influence the properties of the resulting super nanostructure. The range of properties one can get by varying the geometry of nanotube junctions is very wide. Therefore a new area is opened for materials engineers to make versatile materials which will play a significant revolution in almost every engineering field.

2. METHODOLOGY

Using different synthesis methods different types of plane carbon super nanostructures can be formed.

Following (Figs 1-3) are some of the junctions that will be forming during synthesis [3].

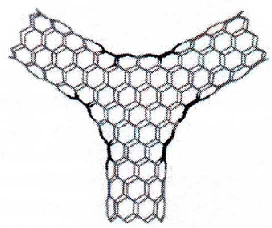

Figure 1. A Y-shaped junction made of zigzag SWCNTs

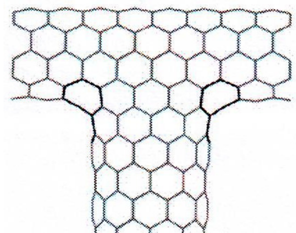

Figure 2. A T-shaped junction made of armchair SWCNTs

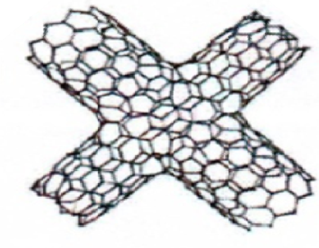

Figure 3. An X-shaped junction zigzag SWCNTs

Different Geometries of Plane super nanostructures

Supergraphenes:

Supergraphenes are formed when the SWCNTs are joined by Y junctions. There can be different geometries in supergraphenes. Some of the extreme geometries are

a) (N,0) supergraphene made of zigzag SWCNTs
b) (N,0) supergraphene made of armchair SWCNTs
c) (N,N) supergraphene made of zigzag SWCNTs
d) (N,N) supergraphene made of armchair SWCNTs.

where N is the chirality of supergraphene or the super carbon nanotube.

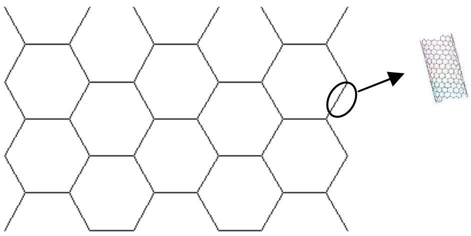

Figure 4. Supergraphene geometry

The elastic properties of these structures can be estimated using simple mechanics model [4] and are found to be varying with C-C bond stiffness, bond length and chirality of the constituent SWCNT as well as with the length and chirality of SWCNT.

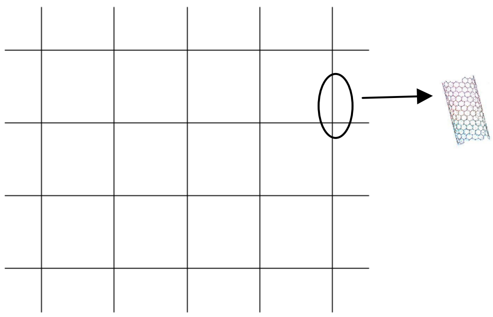

Figure 5. Supersquare geometry

If it is formed by T junctions and cross junctions of SWCNTs then a supersquare structure is formed. It can also be made of zigzag or armchair SWCNTs and the properties will depend on the constituent length and geometry of the supernanostructure. Previous studies on mechanical properties of supersquares were done using molecular mechanics models and impact molecular dynamics calculations [5,6].

Super carbon nanotubes

When the nanotubes are synthesized so that it would form a new orderly nanotube which is made of SWCNTs, it is called a super nanotube. The supercarbon nanotubes can have different geometries and can be manipulated to form a particular structural geometry. A few extreme geometries are;

a) (N,0) Super nanotube made of zigzag SWCNTs
b) (N,0) Super nanotube made of armchair SWCNTs
c) (N,N) Super nanotube made of zigzag SWCNTs
d) (N,N) Super nanotube made of armchair SWCNTs.

These super nanotubes can be again joined to form higher ordered nanotubes which are called hierarchical super nano tubes. Using various geometries almost any desired property can be achieved.

3. RESULTS

Supergraphenes made up from zigzag SWCNTs composed of Y – branches have stiffness (K_{SGX}) values varying from 3,750N/m – 400N/m for the constituent SWCNT length, L_o range of 2nm – 11nm. For the same L_o values the elastic modulus varies from 350GPa – 50GPa (Fig.s 6 and 7).

Zigzag super carbon nanotubes made up from armchair SWCNTs have a stiffness values in the range of 10,000 – 800 N/m for 1 – 6 nm L_o values. For the same L_o values the elastic modulus varies from 600 – 100 GPa and also the ultimate tensile strength from 40 to 5 GPa (Figs. 8, 9 and 10).

To get these results the constituent SWCNTs within the supernanostructures were modeled as linear elastic springs. The C-C bond stiffness, k_{cc} was taken as 831N/m and graphs were plotted for n = 4, 8, 12, 16 and 20 cases as shown in each case.

According to Figure 11 it can be seen that irrespective of the chirality the diameter of the SWCNT is influenced to the elastic modulus of the super carbon nanotube.

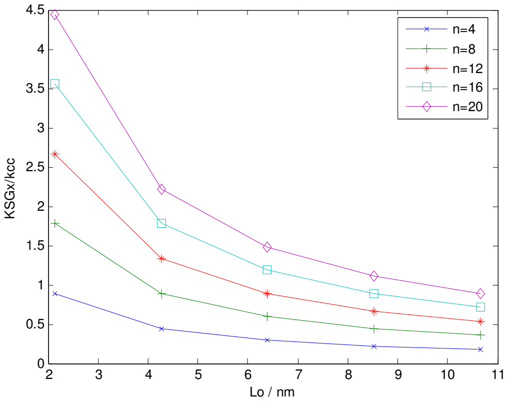

Figure 6. Variation of K_{SGx}/k_{cc} with the length of the constituent zigzag SWCNT where K_{SGx} is the stiffness of [N,0] supergraphene in x direction.

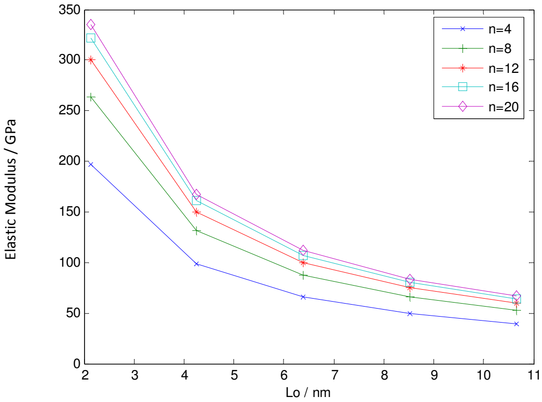

Figure 7. Variation of elastic modulus in [N,0] supergraphene made up of zigzag single walled carbon nanotubes with L_o.

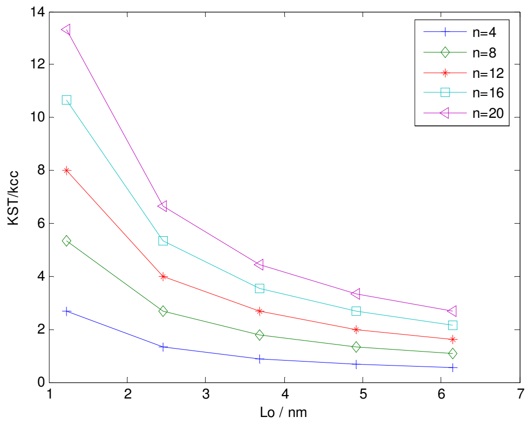

Figure 8. Variation of K_{ST}/k_{cc} in zigzag super carbon nanotube made up from armchair SWCNTs with the length of the constituent SWCNT where K_{ST} is the stiffness of super carbon nanotube in tube direction.

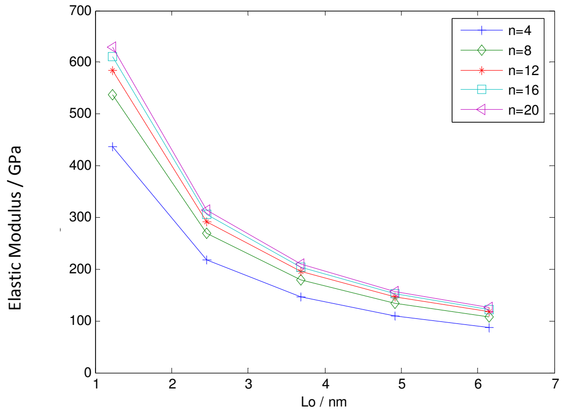

Figure 9. Variation of elastic modulus in zigzag super carbon nanotube made up from armchair SWCNTs with the length of the constituent SWCNT.

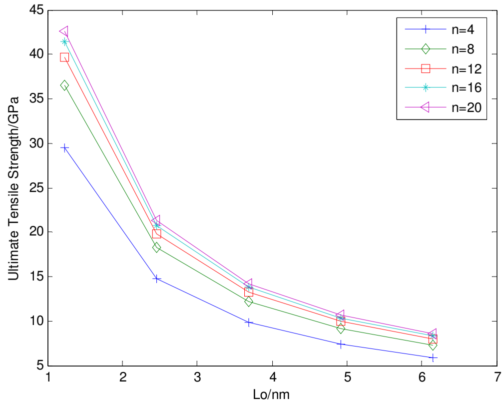

Figure 10. Variation of ultimate tensile strength in zigzag super carbon nanotube made up from armchair SWCNTs with the length of the constituent SWCNT.

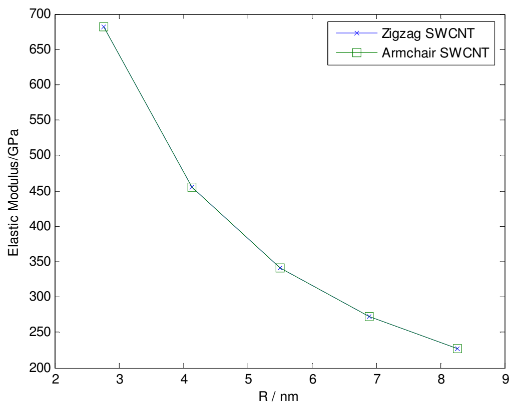

Figure 11. Variation of elastic modulus of zigzag super nanotube with the radius of the zigzag super nanotube for zigzag and armchair SWCNTs.

According to a previous study, it was found that in super carbon nanotubes with Y junctions, the length of the constituent SWCNT and its chirality are influencing the elastic modulus, stiffness and its ultimate tensile strength. Further the study shows that the higher the length of SWCNT the lesser the elastic modulus, stiffness and the ultimate tensile strength. It can be seen that for any type of SWCNT the strength depends on the diameter of the constituent SWCNT, i.e. for both armchair and zigzag SWCNTs the elastic modulus of the super nanotube turns out to be the same. Due to the fact that for a unique chirality in SWCNT the diameter is higher in armchair SWCNT, the strength will be higher in the super carbon nanotube of the (*N*,*N*) armchair geometry than in the super nanotube with (*N*,0) zigzag nanotube [4].

4. CONCLUSION

By manipulating atoms to form different structures, it is possible to obtain different geometries of nano structured materials. These new materials can be mastered to have desired material properties in any range. Therefore these can be used to make bullet proof clothes and vehicles, high strength composite materials, nano electromechanical devices (NEMs) etc. At the same time these low density, flexible materials can be used as light weight materials.

5. REFERENCES

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