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CARBON-CHALCOGENIDE NANOTUBE CONFIGURATION

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New nano-configuration has been modelled, based on nano-tubes of carbon and arsenic sulphide. The properties of this complex structure have been analysed. The modelling shows that the construction of composite nano-structures in different nano-systems are possible.

Key words : Carbon nanotube ; Fullerene; Chalcogenide; As_2S_3 – nanotube, Modelling.

1. INTRODUCTION

The nano-objects are important for the technological development in the field of solid state nano-devices [1-8]. Recently, a growing interest was paid to fullerene – like objects. The synthesis of of fullerene-like and nanotubes made of inorganic layer materials have been tried. For instance, boron-nitride nano-tubes were syntthesized [9] and many of the experiments performed on carbon nano-tubes have been repeated on this system as well [10,11]. Other class of inorganic nanostructures is represented by the vanadium oxide nanotubes [12] Self assembled single wall, sub-nanometer diameter, molybdenum di-sulphide tubes (n-MoS_2) were prepared and investigated [13,14]. Very recently, there were observed nanotubes based on As_2S_3, as a product of the metabolism of the bacteria species *Shewanella* sp. strain HN-41 [15].

The complex nano-configurations based on different material compositions are important for getting new flexible nano-objects to be used in micro and nano-devices. The new functionality of these objects is challenging for the future nano-technology.

We have tried in our research to built a complex configuration with carbon nano-configurations and arsenic sulphide nano-tube, to prove its stability and to look for the possible new properties of use in controllable micro and nano-devices.

2. MODELLING PROCEDURE

In order to model a given structure at nano-scale we started with the building of a network of atoms by interconnecting plastic units that simulate the atoms and their valence directions. Every sulphur atom exhibits two valency directions (two legs). Every arsenic atom exhibits three valence directions (three legs). The carbon unit has been simulated as a triangular planar configuration with three valence directions at 120 ^{o}.

The coordinates of the simulated atoms of the hand-built clusters have been measured directly on the 3D physical models. The coordinsates and the first coordination sphere of every atom were tabulated and been used as input data in a dedicated program for the minimization of the free energy of the structure. The equilibrium distance between As and S atoms was taken 0.225 nm, the bond angle on sulphur was taken 106^{o} and the bond angle on arsenic was taken 98.7, as shown by Rubinstein and Taylor [16]. The nanocarbon tube configuration was built in the same way with trivalent (graphite) atoms with the valence directions at 120^{o} and carbon-carbon bonding distance C-C=1.421 Å. A fullerene with 60 carbon atoms has been, also, built.

The structures of minimum free energy have been calculated by an iteration procedure based on a Monte-Carlo-Metropolis method by using the rule of minimization of the distortion energy (this is called energy relaxation) of the whole model. The free energy of the bonds was calculated by using the force constants given in the literature. The two components of the bonding force are the bond stretching and the bond bending components with appropriate constants of interaction. The bond stretching potential centered on As-S equilibrium distance (r_o) and the bond bending potential was centered on the equilibrium bonding angle of As and S (α_o) [17, 18]

$V_1 = A(r^2 - r_o^2)^2$ with $A = 2.4 \times 10^{-5}$ dyn/Å^3
$V_2 = B(\alpha - \alpha_o)^2$ with $B = 2.04 \times 10^{-4}$ dyn. Å/rad.

The carbon nanotube configuration has been built in the same way and the energy relaxation was carried out with the equilibrium angle of 120^o and bond stretching and bond bending force constants of 0.605×10^{-03} dyn/Å^3 and 0.047×10^{-03} dynÅ/rad^2, respectively [20].

3. RESULTS

Firstly, we modeled an arsenic sulphide nanotube configuration with 214 a toms (As+S). The nanotube exhibited open ends. In this case at the ends there are dangling bonds. A nanotube made of carbon atoms was built with open ends, as in the previous case. Thus it is possible to interconnect in a natural way nanotubes with different compositions.

We have tried to built a structure consisting of an arsenic sulphide network of atoms, known to have a nanotube structure and, at one end a carbon nanotube and at the other end a fullerene ball.

After interconnection, we have relaxed the complex nano-object based on carbon nanotube – As_2S_3 nanotube- fullerene ball (C_{60}). The carbon nanotube is a zig-zag nanotube (15,0). At the right hand side the nanotube end is formed by 2 × 5 rings of 5 carbon atoms. At the lieft hand side, the nanotube of As_2S_3 is a"zigzag" configuration (5,0), that connects the fullerene C_{60} ball lacking one 5 fold ring of atoms. The free energy / (bond and angle) of 2.668 meV was found after relaxation.

Fig. 1 shows the final configuration after energy relaxation, the distance distribution in the model (a), the structure factor (b) and the bonding angle distribution (c).

Fig. 2 illustrates the variation of the free energy of the configuration along the nanotube axis. In the region of connection carbon nanotube-arsenic sulphide tube, the distortion energy is very high (5 meV). In the connecting region nanotube-fullerene the distortion energy changes by about 1.5 meV.

A preliminary report on the construction and relaxation of this nanostructure has been done in Reference [19].

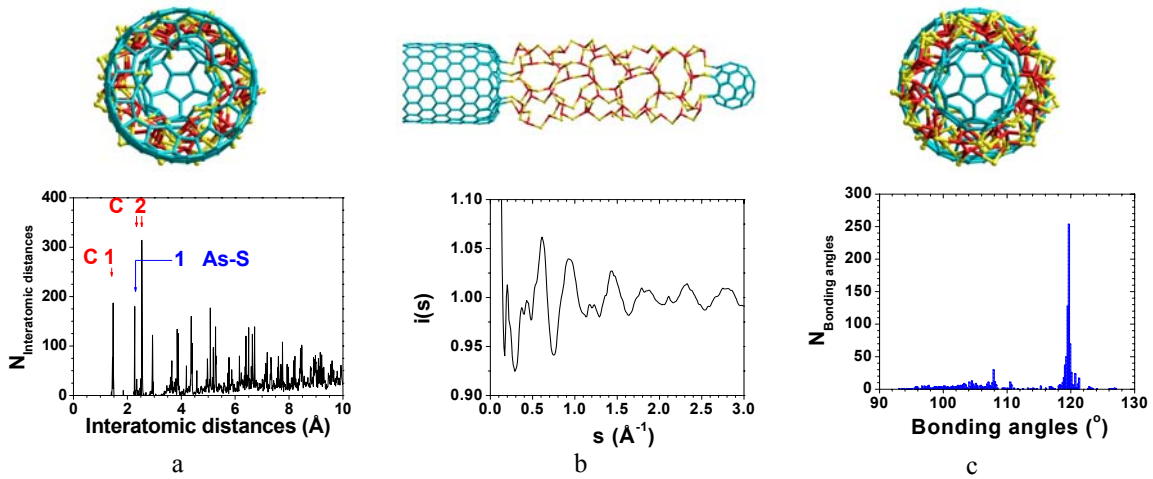

Fig. 1 – Carbon nanotube with zig-zag configuration (15, 0), having at the coupling end 2 pentagonal rings of atoms linked to a zig-zag arsenic sulphide nanotube. At the other end of the zig-zag arsenic sulphide tube a fullerene molecule is attached. For making the connection one 5-fold rings of atoms was eliminated.

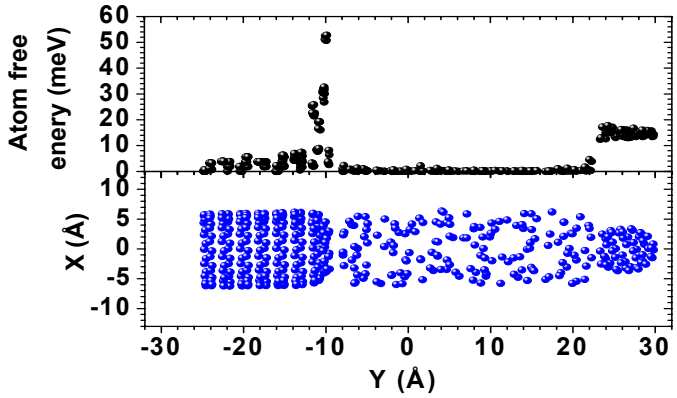

Fig. 2 – The distribution of the distortion energy in the complex nanostructure based on the combination of a carbon nanotube, an As_2S_3 chalcogenide nanotube and a fullerene C_{60} molecule.

4. DISCUSSION

The first observation is related to the equilibrium of the distortion energy in this complex configuration. This fact speaks in favour of the chemical stability of this nano-object. On the other hand, as a consequence of stable chemical structure it is possible to exploit different properties of the parts of the complex configuration. For example, the fullerene filled by atoms, as e.g. Rb, or complex K-Rb molecules can control the superconductive properties at very low temperatures. The arsenic sulphide nanotubes can exploit the interaction with light. The chalcogenide are very sensitive to light: The photo-expansion and photo-contraction effects can trigger the transmittance of the charge carriers or atom transit through the complex configuration. The doped nanotubes can serve as nanowires in micro and nano-devices. One challenging property of the complex is the high distortion accompanied by high electrical field in the junction region between nanotubes. This gate could be of interest for triggering the access of charge carriers from one nanotube to another. By fine control of the carrier transport, a rectifying system can be imagined

Recently, we have demonstrated the gas sensing effect in complex configuration of barium stearate molecular fatty chains and single wall nanotubes. The mixture at nanoscale and possible alignement of nanotubes along the fatty acid molecules makes the system efficient in sensing the NO_2 gas. The sensing is based on the significant diminishing of the electrical resistivity with the increase of gas concentration. A resistivity diminishing of ~6 % for 2.5 ppm concentration of NO_2 in air makes the system applicable in sensor devices with very high detectivity.

5. CONCLUSIONS

It is a challenge for chemists and physicists to prepare new materials at the nano-scale, based on low coordinated elements as e.g. P, As, S, Se , Te, etc.

The modeling is useful for choosing the best configurations to be tried experimentally. Our study demonstrates the feasibility of a connection carbon nanotube – As_2S_3 nanotube of interest in conjunction with the light excitation for the control of the carrier transport in the nanoscale devices.

The new materials could be a reservoir of new properties and applications in nano-technology.

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