MODELLING OF THE COMPLEX CARBON STRUCTURE: FULLERENE – NANOTUBULE

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The complex structure fullerene(C_{60})-nanotubule has been built from special plastic units and relaxed by a computer Monte-Carlo – Metropolis procedure. The purpose was to show that interconnection fullerene-nanotubule is possible from the energetical point of view. The results open the way towards the assessing the possibility to create nano-conductors and connections between different parts of nano-devices, using nano-carbon configurations filled by metal atoms.

The structure of the carbon nano-configurations is still poorly known and understood. Some basical configurations have been discovered, as e.g. ball-like fullerenes with various number of carbon atoms [1], nanotubules of various radii [2], onion-like carbon [3], etc... The nano-carbon species attracted the attention of the researches in nano-devices, due to their possible use in the building of nano-conductors by filling e.g. the nanotubules by metallic atoms. The alkali metals have been introduced in the fullerene C_{60} and it became superconducting with a maximum superconducting temperature of 33 K [4]. Lozovanu et al. [5] have pointed out the photo-luminescence properties of fullerene C_{60} thin films, and they demonstrated that the luminescence effect is given by the impurities.

On the basis of past experience in modelling the amorphous nano-structures [6,7] we have started a program of modelling the nano-configurations of the newly discovered carbon species in order to see if new carbon configurations could be prepared and metallic atoms could be inserted in order to create nano-conducting wires, to be used in nano-devices. We report here the first results on modelling of the combination C_{60} fullerene with a nanotubule of small diameter.

The starting point was the building of two basical models: a fullerene ball with 60 atoms and a nanotubule with 154 atoms. The relaxed configurations are represented in Fig. 1a,b.
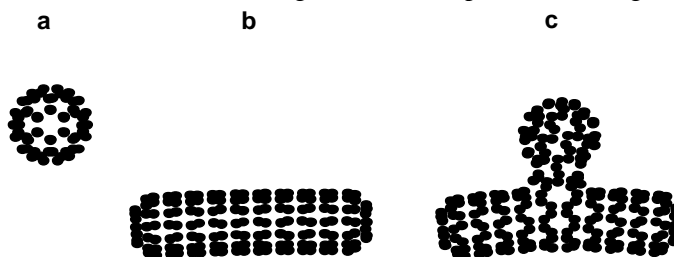

Fig. 1. Relaxed model of the fullerene C_{60} (a), nanotubule (b), fullerene-nanotubule (c).

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Both configurations have been relaxed in the frame of the valence force field model [8] and bond stretching and bond bending force constants as given by Martin [9]: $k_r = 2.375 \times 10^{-5}$ dyn/Å^3 and 2.063×10^{-4} dyn.Å, respectively.

The calculation of the free energy of every carbon configuration was carried out by the Monte Carlo – Metropolis method, with special computer programs developed in the National Institute of Materials Physics, and run on powerful PC computers. For every configuration there were performed 60 millions iterations, starting with the working step of 0.02 nm and gradually reducing this step in order to refine the structure.

An important stage of the modelling was the building of the complex structure fullerene-nanotubule (214 atoms), by connecting the ball configuration on the middle part of the nanotubule. The structure was relaxed by the same computer procedure and the result is shown in figure 1c. The aim was to show that such a structure is physically realistical and, therefore, could be suggested to play the role of the interconnection wires between nanodevices.

The analysis of the angles between bonds in the models show that in the fullerenes the angles are distributed around two peaks of 108° and 120°, corresponding to the 5 and 6 atoms rings characteristic to C_{60}. The root mean square deviation is 5.679° for every type of ring. The bonding angles in the carbon nano-tubule correspond to 108° and 119°. The root mean square deviation of the bond angle is 3.926°. The deviation from the graphite bond is due to the curving of the layer that forms the nanotubule.

In the complex structure fullerene-nanotubule the distribution of the bonding angles is significantly distorted (rms = 4.718°) but not overcomes the distortion in C_{60} fullerene. The distance between atoms is situated near the ideally one (0.1468 nm) and rms is 0.0013 nm. The average second order distance between atoms is 0.2880 nm and the dispersion is 0.0202 nm. An important result of the modelling is the effect of curving the nanotubules by attaching the ball fullerene ball at its wall (see fig. 1c). The curvature is determined by the formation of very distorted bonds at the surface of the complex.

In order to have a tool for the identification of the complex fullerene-nanotubule in the experimental samples, we have calculated the X-ray diffraction patterns (or interference patterns) on the three relaxed models. The results are shown in Fig. 2 a-c.

The complex configuration is characterised by a high peak situated at $s = Q/2\pi \sim 8.42$ nm^{-1} while for the simple configurations this peak is shifted to 8.92 nm^{-1} for fullerene and 8.44 nm^{-1} for nanotubule. The fullerene C_{60} exhibits also a characteristic peak to 3.3 nm^{-1}.
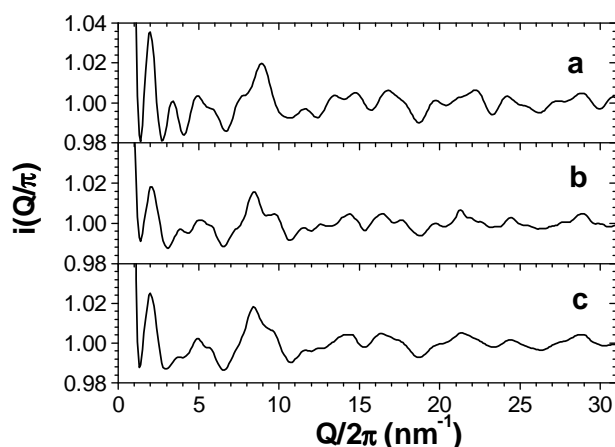

Fig. 2. The X-ray diffraction patterns (structure factor) calculated for the three configurations of the carbon. a. fullerene C60; b. nanotubule (154); c. complex fullerene - nanotubule (60+154).

Further, we have investigated the dihedral angle distribution in the three models of nano-carbon species (Fig. 3). The distribution of the dihedral angles in fullerene (C_{60}) is: 180 angles with

0°, 60 angles with 138° and 120 angles with 142°. For the nanotube the dihedral angles show a larger dispersion due to the closed ends: 126 angles with 0°. and 224 angles with 26°. New angles appear at 4° (28 angles) at 6° (56 angles) and at 10° (28 angles). In the fullerene-nanotubule complex the dihedral angles are distributed on a larger range with maxims at 0°, 2°, 6°, 10°, 26°, 128°, 138° and 180°. This means that the complex configuration is subjected to inhomogeneous stresses. The identification of these stresses is important. The preliminary determinations have shown that the junction fullerene-nanotubule is the most distorted one: the stresses are the largest.
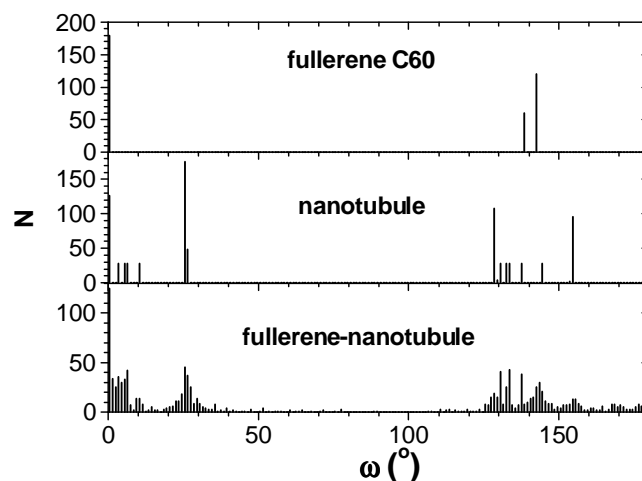
Fig. 3. Dihedral angle distribution in the three relaxed models of nano-carbon configurations.
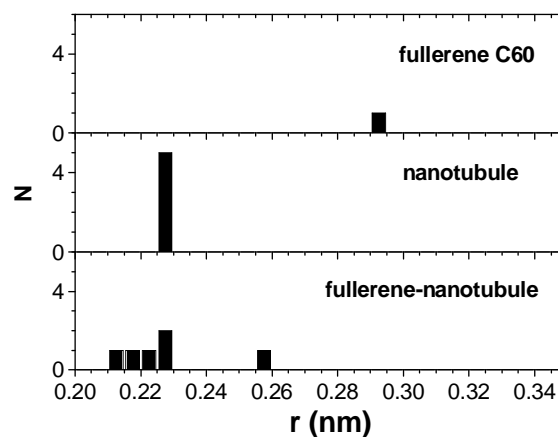
Fig. 4. Void distribution in the three relaxed models of nano-carbon configurations.

Finally, the void structure of the carbon configurations has been studied. Fig. 4 shows the results. In the normal fullerene (C_{60}) the unique void radius is 0.2925 nm. The nanotubule contains a void of diameter 0.2275 nm, while the complex fullerene-nanotubule contains a distribution of voids situated between 0.2125 and 0.2275 nm.

The conclusion of the modelling studies are: a. the nanometric structure of the combination fullerene-nanotube is physically realistic b) the bonding distortion at the junction fullerene – nanotube is enough low to permit the coupling of the fullerene molecule to nanotubule, c). the structural voids in the complex are enough large to permit the introduction of the metallic atoms (Fe, Co, Ni /r_{av} ~0.123 nm) to form compact rows, or small clusters, thus giving rise to metallic conduction; this could be used in the integrated systems based on nano-devices, in the future optoelectronics d). the modelling of the carbon nanostructures is a simple and cheap method and can be easily extended to

other systems, as e.g. silicon, in order to demonstrate the feasibility of nano-wires for applications in nano-electronics and spintronics.

Acknowledgement

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