COMPUTER SIMULATIONS OF CARBON NANO-OSCILLATORS AND THEIR DYNAMIC PROPERTIES INVESTIGATION

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Recently a great theoretical and experimental research effort has been carried out in order to investigate the encapsulation processes and oscillatory mechanisms of C60 and C20 fullerenes into nanotubes [1]. In this work we present the molecular dynamics simulation of oscillation processes in the systems of a C60 fullerene and a single walled armchair (12,12) carbon nanotube. The two different configurations of the system were considered. Our results show that these devices are dynamically stable; frequencies about 1 THz were observed. In addition, more complicated type of interaction between the nanotube and the C60 fullerene was noticed.

1 Introduction

Today carbon nanotubes are considered as the basis for a new generation of electronics, which is significantly faster than the modern silicon one. It is the unique properties of such systems which further it [2].

Computer simulation, particularly, molecular dynamics, plays a significant part in the investigation of nanomaterials and nanoobjects, as it allows to obtain in-depth information about time evolution and dynamics of many physical nanoscale processes.

In this paper it is presented simulations of processes in two different configurations: 1) the quasi axial oscillations of the C60 fullerene into the single walled armchair (12,12) carbon nanotube; 2) the radial oscillations in the system of the C60 fullerene and a short fragment of carbon nanotube (12,12).

2 Methodology

We have carried out molecular dynamics simulations using the ChemBio3D application in the framework of classical mechanics with a standard molecular force field which includes van der Waals, bond stretch, bond angle bend, and torsional rotation terms.

The main features of calculation the Van der Waals Energy in Chem3D. Repulsive forces dominate when the distance between interacting atoms becomes less than the sum of their contact radii. In Chem3D repulsion is modeled by an equation which combines an exponential repulsion with an attractive dispersion interaction ($1/R^6$):

$$E_{VdW} = \sum_i \sum_j \varepsilon \left(290000 \mathrm{e}^{-12,5\,R} - 2,25\,R^{-6} \right) \tag{1}$$

where

$$R = \frac{r_{ij}}{R_i^* + R_j^*} \tag{2}$$

The parameters include:

- R_i* and R_j*—the van der Waals radii for the atoms,
- Epsilon (ε)—determines the depth of the attractive potential energy well and how easy it is to push atoms together,
- r_{ij}—which is the actual distance between the atoms.

At short distances the above equation favors repulsive over dispersive interactions. To compensate for this at short distances (R=3.311) this term is replaced with:

$$E_{VdW} = 336,176 \sum_i \sum_j \varepsilon R^{-2} \tag{3}$$

In our case it is used the following parameters: ε = 0,046; R^*_i = 3,34 Å; the cutoff distance is 10 Å. All simulations are carried out at T=80 K, without heating.

3 Calculations and results

A. Axial oscillations of the C60 fullerene into the single walled armchair (12,12) carbon nanotube

The structures are generated in the following way. The coordinates of single chain atoms of carbon nanotube (12,12) are calculated taking into consideration the bond length and the structure. The tube is constructed up to 21 Å. Then the C60 fullerene is displaced in alignment with the nanotube.

This construction consists of 492 carbon atoms.

Constituent of constructed system – carbon nanotube (12,12) and C60 fullerene, diameters of which are 16,27 Å and 7,1 Å, respectively, were chosen taking into consideration the distances on which the Van der Waals forces act.

The initial position of the C60 fullerene was chosen such that it can be attracted by the nanotube and subsequently be entirely encapsulated into the nanotube.

At the next step the constructed system is undergone the molecular dynamics simulation.

A time step of 4 femto seconds is used for this simulation.

The atoms of the nanotube were frozen for the purpose of speeding-up the calculations. This assumption warranted by the fact that breathing of the nanotube has a weak influence on the motions of the C60 fullerene in it; and in reality vibrations of the nanotube will dissipate on junctions or substrate of a device.

The C60 fullerene begins to move into the nanotube under the Van der Waals force. When it reaches the opposite nanotube end (Fig.1), its velocity vanishes and the fullerene returns to the nanotube interior, forming then a nanooscillator.

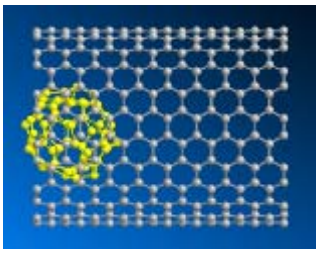

Fig. 1 The C 60 fullerene reaches the opposite nanotube end, its velocity vanishes

Our calculations show that period of observed oscillation is 18,400 fs, and consequently its frequency is $0{,}054*10^{12}$ Hz.

As a result of detailed investigation more complicated type of interaction between the nanotube and the C60 fullerene was noticed (Fig.2).

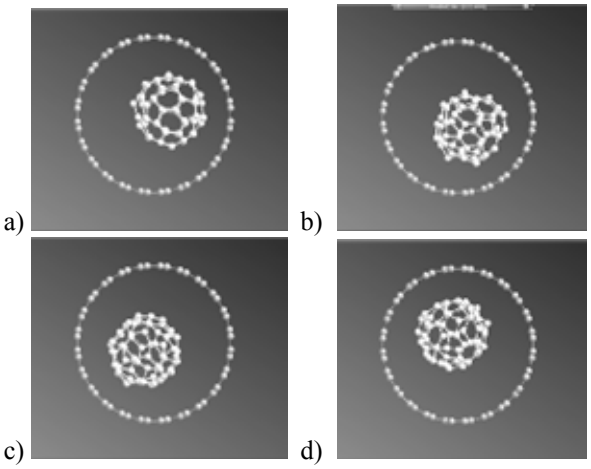

Fig.2 Quasi axial movement of the fullerene in the nanotube

Firstly, the C60 fullerene moves along the tube axis and oscillates in radial direction ($14*10^{10}$ rps) as well. Therefore this motion is actually quasi axial one. Secondly, during the quasi axial movement the C60 fullerene rotates on its axis (maximal rotation is 40˚-50˚). These findings indicate the more fine details of nanooscillator energy state, which is due to the certain anisotropy of the interaction between the C60 fullerene and the nanotube wall.

Yang Zhao et al. performed simulations on (5,0)/(14,0), (7,7)/(12,12) and other DWNT oscillators and it is shown that a DWNT oscillator with thousands of degrees of freedom can be reduced to a simple system with a few most relevant degrees of freedom in the presence of a thermal bath. Those few degrees of freedom correspond to several important low-frequency mechanical modes such as intertube axial oscillation, intertube rotation and bending-waving modes while the thermal bath is made of other higher-frequency vibrations of the nanotube. When the energy leakage from the reduced system to the bath is slow enough, the reversible energy exchange between the oscillator and the bending-rotational modes takes place thanks to the reduction of the effective phase space [3].

B. Radial oscillations in the system of the C60 fullerene and a short fragment of carbon nanotube (12, 12)

Further we interested in creation of the system with higher frequency oscillations. For this purpose we simplified previous construction and studied the dynamics of a new received system in which radial oscillation is dominant.

This new configuration of the system is generated in the following way.

A short fragment of carbon nanotube is constructed up to 4,93 Å length. Then the C60 fullerene is displaced in the center of this fragment in the way shown in Fig.3.

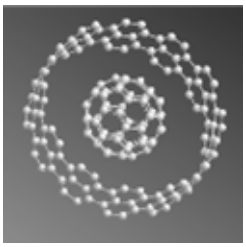

Fig. 3 System of the C60 fullerene and the fragment of nanotube

The whole of the construction consists of 180 carbon atoms. This system is also calculated using the classical molecular dynamics method. Time step is 0.5 fs. Fixed temperature is 80 K.

As a result the radial oscillation of the nanotube fragment was observed (Fig. 4).

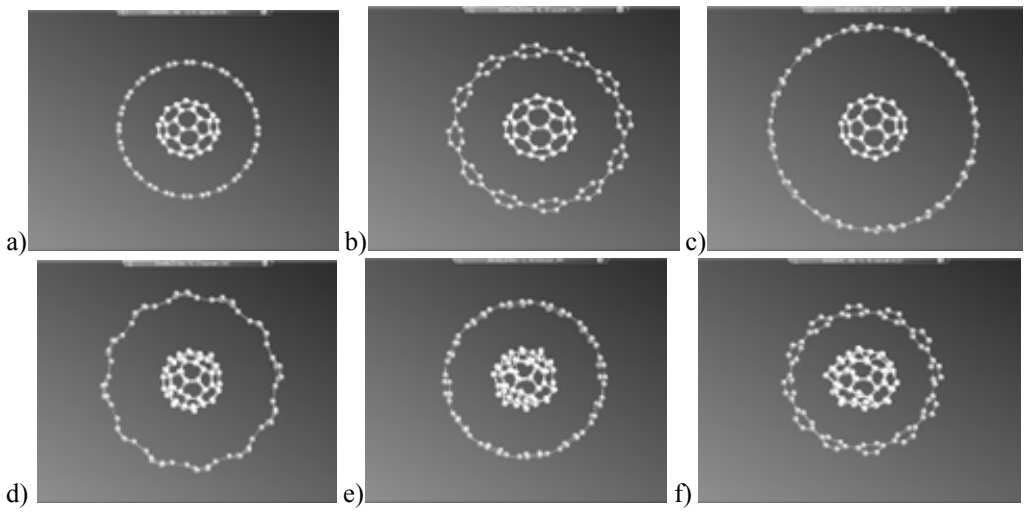

Fig. 4 Time evolution of the system of the C60 fullerene and the fragment of carbon nanotube (12,12)

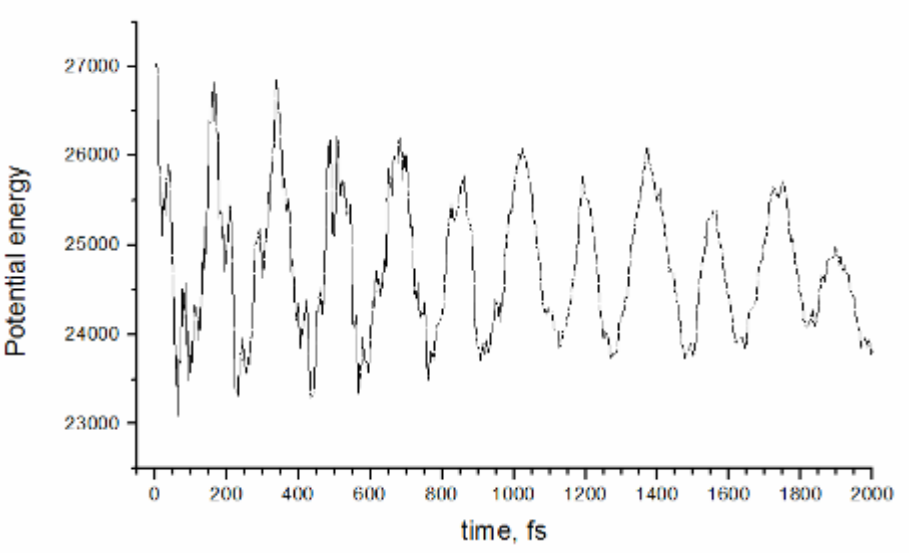

Fig. 5 Potential energy – time curve of the radial oscillator.

In Fig. 5 the peaks of potential energy correspond to the maximum dilatations of the system from the equilibrium position, i.e. maximal compression and stretching of the nanotube.

As a result of calculations the following data was received: amplitude of the radial nanotube oscillation is 4,5 Å (D_{min}=4,32 Å, D_{max}=8,84 Å); frequency of this oscillation is 2,9 *10^{12} Hz.

Thereby we have observed oscillation with frequency of infrared region.

4 Summary

The molecular dynamics simulation was performed for the interaction processes among the C60 fullerene and the carbon nanotube (12,12). The two high-frequency oscillatory systems have been studied.

One concept that has attracted much attention is the creation of nanooscillators, to produce frequencies in the gigahertz range, for applications such as ultra-fast optical filters, nano-antennae and nanomemory devices [4]. The sliding of an inner shell inside an outer shell of a multiwalled carbon nanotube can generate oscillatory frequencies up to several gigahertz, and the shorter the inner tube the higher the frequency[5].

In this work the C60-nanotube oscillator generates nearly terahertz frequency by oscillating the C60 fullerene inside the single-walled carbon nanotube (12,12). Also the frequency in the system of the C60 fullerene and a short fragment of carbon nanotube was estimated.

The sealed devices constitute the ideal configuration and work perfectly. The recent advances in the synthesis, controllable manipulation and chemical etching of carbon nanotubes make the sealed oscillators we are proposing feasible in our present technological capabilities [6].

References

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КӨМІРТЕКТІ НАНО-ОСЦИЛЛЯТОРЛАРДЫ КОМПЬЮТЕРЛІК МОДЕЛЬДЕУ ЖӘНЕ ДИНАМИКАЛЫҚ ҚАСИЕТТЕРІН ЗЕРТТЕУ

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Жақын арада нанотүтікшелердегі С60, С20 фуллерендерінің тербелу механизмі мен инкапсуляциясын зерттеу мақсатында үлкен теориялық және эксперименттік жұмыс жасалады. Берілген жұмыста фуллереннің С60 және бір қабықшалы көміртекті нанотүтікше жүйелерінде тербелу молекулалық динамикалық модельдеу келтірілген. Жүйенің екі түрлі конфигурациясы қарастырылған. Нәтижелердің көрсетуі бойынша, осындай құрылғылар динамикалық тұрақты; жиілігі 1ТГц тербелістер байқалған. Сонымен қоса, нанотүтікшемен фуллерен С60 – тың әрекеттесуінің күрделі түрі анықталды.

КОМПЬЮТЕРНОЕ МОДЕЛИРОВАНИЕ УГЛЕРОДНЫХ НАНО-ОСЦИЛЛЯТОРОВ И ИССЛЕДОВАНИЕ ИХ ДИНАМИЧЕСКИХ СВОЙСТВ

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Недавно была произведена большая теоретическая и экспериментальная работа в целях исследования процессов инкапсуляции и колебательных механизмов фуллеренов С60 и С20 в нанотрубках. В данной работе мы представляем молекулярно динамическое моделирование колебательных процессов в системах из фуллерена С60 и одностенной углеродной нанотрубки (12,12). Были рассмотрены две различные конфигурации этих систем. Результаты показали, что подобные устройства динамически стабильны, наблюдались колебания с частотой около 1 ТГц. Кроме того, был обнаружен более сложный тип взаимодействия между нанотрубкой и фуллереном С60.