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Investigation of the state of C_{60} @ CNT in the presence of an electric field

D. Karastoyanov[1], *A Bubenchikov*[2], *M Bubenchikov*[2]

D Mamontov[2] *A Lun-Fu*[3]

[1]Institute of Information and Communication Technologies – BAS

[2]Departamenf of mechanics, Tomsk State University, Tomsk 634050, Russia.

[3]Gazprom transgaz Tomsk, Tomsk 634029, Russia.

Email: orevaore@mail.ru

Abstract. *The paper presents a mathematical model for numerical simulations of rotating fullerenes in carbon nanotubes of various chiralities. The analyzed natural rotations of C_{60}@CNT, as well as regular and oriented rotations due to the action of an external electromagnetic field harmonically varying in time. Calculations show that oriented rotations can only be achieved in the case of initially centered C_{60} with respect to CNT.*

Keywords: *Fullerenes, carbon nanotubes, mathematical modeling, molecular mechanics.*

1. Introduction

Carbon is the foundation of life on Earth. Therefore, bio-medical studies of nanocarbon are of great importance in the creation of artificial carbon fragments, their implantation in living systems, as well as in the survival of these fragments in biological systems. Along with these applications, the technical applications of nanocarbon, as well as the development of new materials based on it, are gaining importance. Fullerite is a versatile material with great potential for use in various fields. To determine the properties of this material, the vibrational – rotational spectrum of molecular hydrogen in a fullerite crystal was studied in [1]. Standard fullerene - C_{60} is the most advanced carbon molecule with icosahedral symmetry and therefore deserves special attention. At the same time, studies of the state of even larger carbon molecules remain important: fullerenes, graphenes, carbon nanotubes. In [2], the stresses in the graphene sheet were determined by the action of standard fullerene on it. Data were obtained by [3] on the mechanical and chemical interaction of large fullerenes with defective graphene. [4] demonstrated the dynamic state of a cluster consisting of 27 C_{60} fullerenes was simulated. In [5], using the Tersoff potential, the frequency characteristics of the group of the most famous fullerenes were calculated. In [6], using the molecular dynamics models, the thermal and dynamic characteristics of the onion complex $C_{20}@C_{80}$ are analyzed. The technology for wrapping fullerenes with graphene sheets was considered in [7]. The authors [8], based on the Tersoff potential, vibrational modes of crystal lattice sites in fullerenes of various masses are considered. In [9], the vibrations of fullerenes near a graphene sheet were studied. [10] described the magnetic properties of sulfonated fullerene are analyzed. The synthesis of triblock derivatives of fullerenes is described in [11]. In [12], a nanocomposite for applications in solar cells was obtained. To date, water-soluble fullerenes have already been synthesized [13], which have broad prospects for medical applications. Conventional fullerenes are already used in medical research [14]. The long stage of stellar life is associated with carbon synthesis; therefore, fullerenes were recorded in open space [15]. On Earth, fullerenes are found in the atmosphere and in meteorite matter [16, 17]. The comprehensive distribution of fullerenes is of great interest in the study of materials created on their basis. In [18], the physical properties of some nanocomposites reinforced with fullerenes, as well as carbon onion structures, were considered. The magnetization of fullerenes was considered in [19]. In [20, 21], data on the vibrations of the shells of fullerenes C_{30} and C_{60} are presented. In [22], the design design of a new fullerene-graphene material was performed. In [23], the idea of a new material based on fullerite with ultrahigh stiffness was discussed. In [24], diffusion of a molecule of high molecular potential, in particular, C_{60}, was considered.

2. Mathematical model and calculation details

2.1. Forces of cross atom-atom interactions

It is known that the interaction of C_{60} molecules in fullerite is of Van der Waals nature and can be modeled through atom-atom interaction. The magnitude of

the force acting on an individual atom of the C_{60} molecule can be determined if the carbon-carbon interaction potential is known. In this case, the force will be the potential gradient taken with the opposite sign.

Sometimes, for fullerenes, the potential of intermolecular interaction is used, while it is usually smoothed out. However, such a centrally symmetric potential does not provide the natural rotation of fullerenes. The first approximation of the real pair potential of fullerene interactions can be the potential of cross atom-atom interactions (interactions realized between atoms belonging to different fullerenes).

$$X_k = -\sum_{j=1}^{N_p} \frac{\partial U}{\partial x}\left(r_{kj}\right), \tag{1}$$

$$Y_k = -\sum_{j=1}^{N_p} \frac{\partial U}{\partial y}\left(r_{kj}\right), \tag{2}$$

$$Z_k = -\sum_{j=1}^{N_p} \frac{\partial U}{\partial z}\left(r_{kj}\right). \tag{3}$$

Here X_k, Y_k, Z_k – re the projections of the resultant of all forces (acting on the kth atom of the molecule under consideration from other fullerite atoms) on the axis of the fixed reference frame, $r_{kj} = \left|\boldsymbol{r}_k - \boldsymbol{r}_j\right|$, $\boldsymbol{r}_k$ – is the radius vector of the *k*-th atom of the central molecule C_{60}, r_j is the radius vector of the *j*-th atom of the surrounding molecules, N_p is the number of carbon atoms in the minimum fragment of the face-centered structure with the exception of the atoms of the central fullerene, $U(r_{kj})$ is the atom-atom interaction potential

2.2. Rotation of fullerenes in the presence of electromagnetic fields

The dynamic Euler equations for the projections of the angular velocity on the axis associated with the rotating fullerene in this case have the form:

$$A\frac{dp}{dt} + \left(C - B\right)qr = M_{\xi} + M_{\xi}^{(m)} + M_{\xi}^{(e)}, \tag{4}$$

$$B\frac{dq}{dt} + \left(A - C\right)pr = M_{\eta} + M_{\eta}^{(m)} + M_{\eta}^{(e)}, \tag{5}$$

$$C\frac{dr}{dt} + \left(B - A\right)pq = M_{\zeta} + M_{\zeta}^{(m)} + M_{\zeta}^{(e)}. \tag{6}$$

Here the quantities with the superscript «*m*» are the projections of the moments of magnetic forces on the moving axes, and with the index «*e*» - are the projections of the moments of electric forces on the same axes; *p*,*q*,*r* – are the projections of the angular velocity on the moving axes associated with the rotating fullerene; *A*,*B*,*C* – are the main moments of inertia of the molecule for its center of mass. These equations are closed by the kinematic relations of Euler.

2.3. Displacements of the centers of mass of molecules

The equation of motion of the centers of mass of polyatomic molecules within the framework of the description used for cross atom-atom interactions is calculated as follows:

$$M\frac{d\boldsymbol{v}_C}{dt} = -\sum_{j=1}^{N_p}\sum_{k=1}^{S}\nabla U\left(r_{jk}\right) + \boldsymbol{E}q. \qquad (7)$$

Here M – is the mass of the molecule, $\boldsymbol{v}_C$ – is the velocity of the center of mass of the moving molecule, S – is the number of atoms in the molecule, ∇ - is the gradient operator, $\boldsymbol{E}$ - is the electric field vector, q - is the fullerene charge. As we see from (7), the motion of the center of mass of a polyatomic molecule is determined by the effect of all environment atoms on each atom of the molecule, as well as by the action of the electric field.

3. Results of calculations

In all calculations, the magnetic field was constant, and the electric field was harmonically changing and flat $E_x = a\cos 2\pi ft, E_y = a\sin 2\pi ft, E_z = 0.$ Ordinary differential equations that determine both the rotational and translational movements of fullerenes are integrated numerically using high-precision methods of step-by-step integration. As a result of solving the problem, the trajectories of all atoms of all fullerenes were determined. In fig. 1 shows a variant of the free motion of fullerene in an electric field of a given configuration. In this case, the trajectory of the charged node on the fullerene is circular. However, due to the inertia of fullerene, its rotation frequency, in contrast to the frequency of the electric field, is not a constant value, but varies according to a harmonic law.

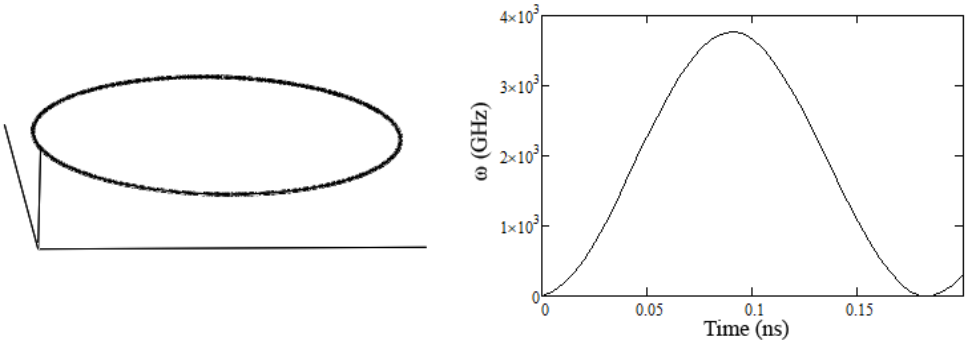

Figure 1. Circular rotation of fullerene in a harmonically changing electric field.

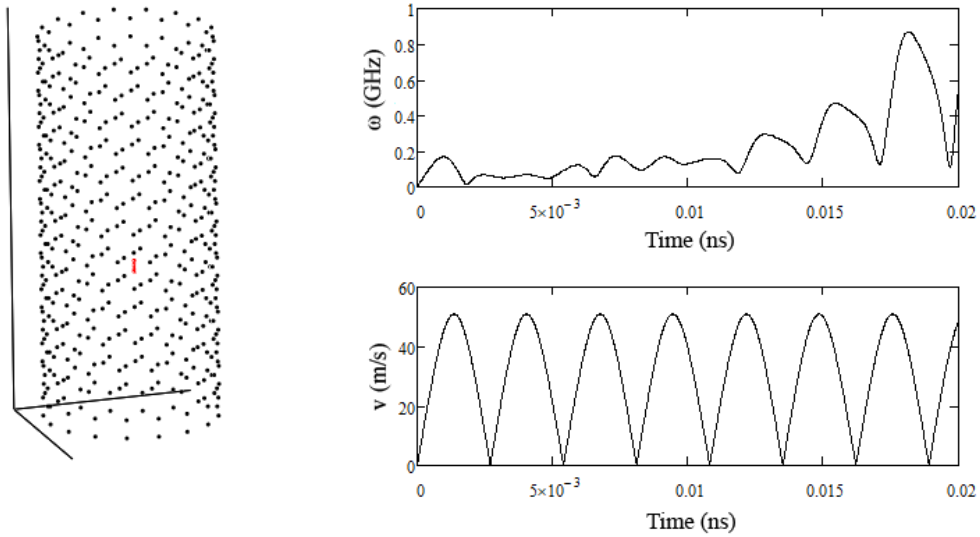

Figure 2. Natural rotation of centered fullerene C_{60}@CNT (17,0), no electric field.

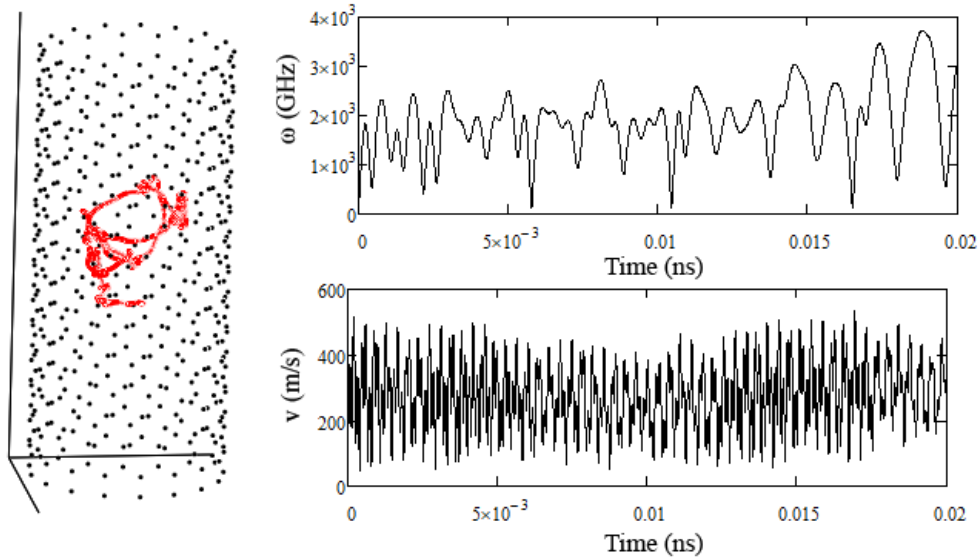

Figure 3. Regular rotation C_{60}@CNT(17,0), in an electric field a=10 kV/m, f=1000GHz.

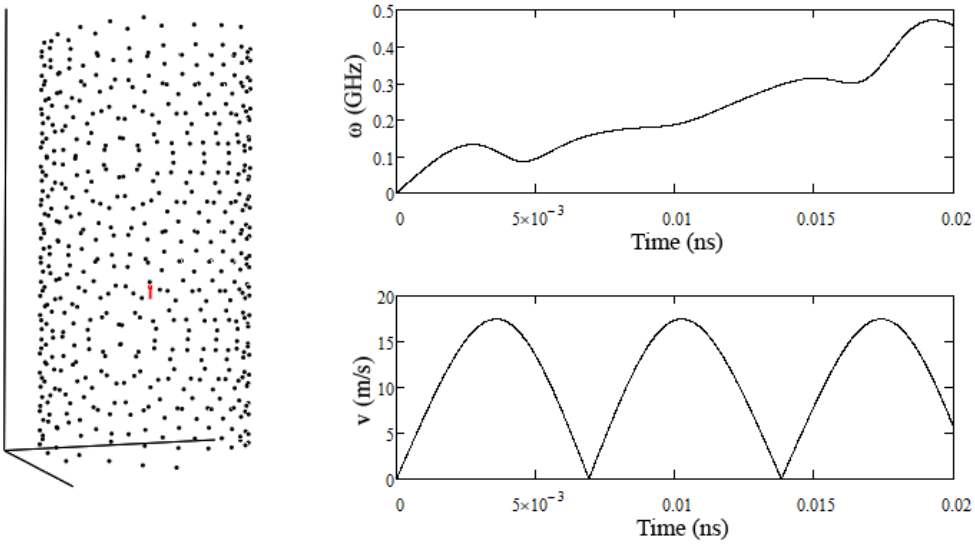

Figure 4. Natural rotation of fullerene C_{60}@CNT(18,0), there is no electric field.

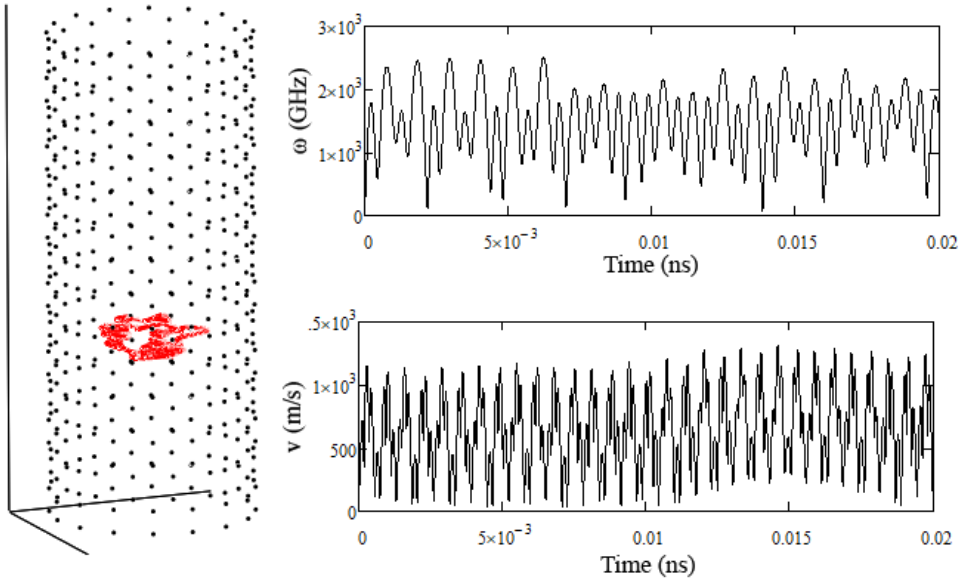

Figure 5. Fullerene C_{60} spun by an electric field: a=10 Kv/m, f=1000 GHz, inside the CNT(18,0) (diameter 1.4 nm).

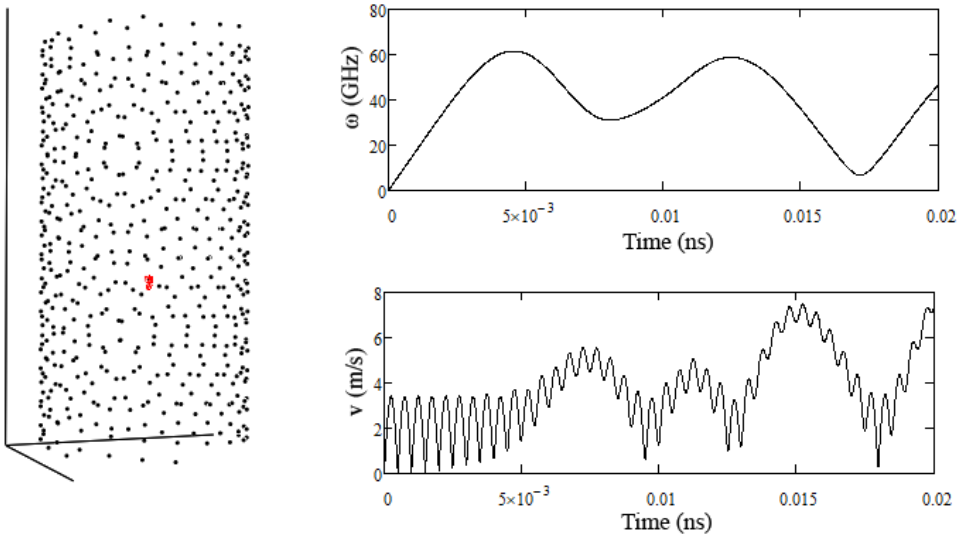

Figure 6. Natural vibrations C_{60}@CNT(16,4)

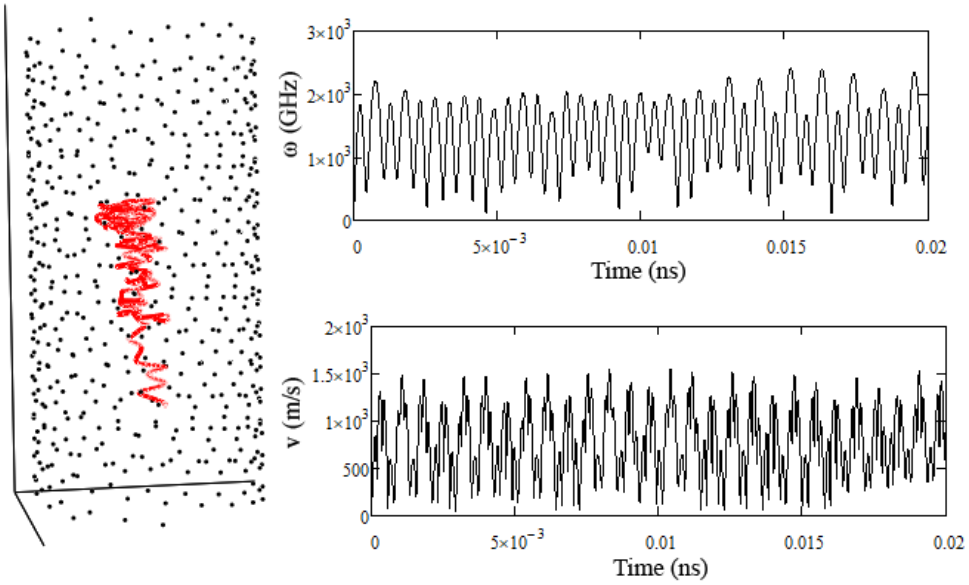

Figure 7. Rotations C_{60}@CNT(16,4) in an electric field a=10 kV/m, f=1000 GHz.

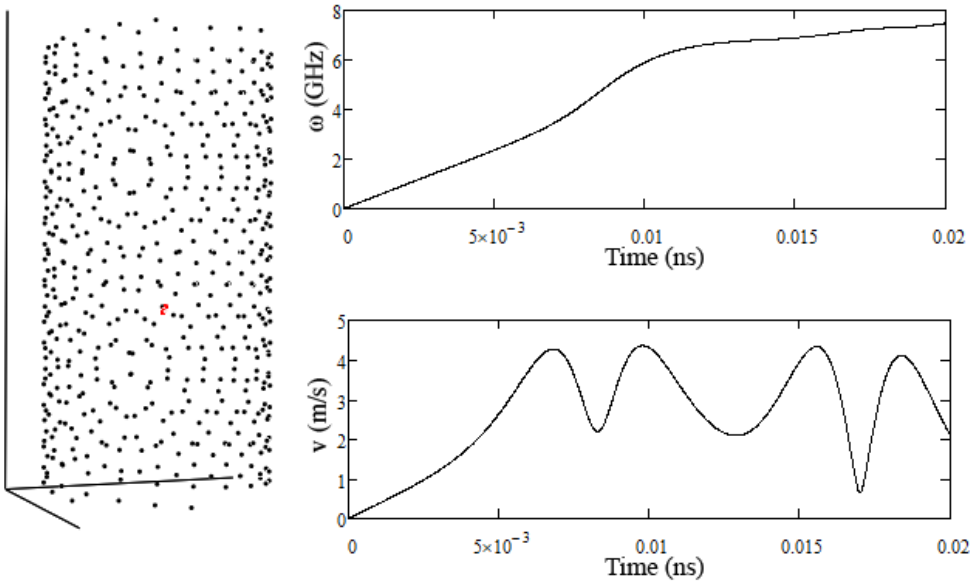

Figure 8. Natural vibrations C_{60}@CNT(18,2) in the absence of electric fields.

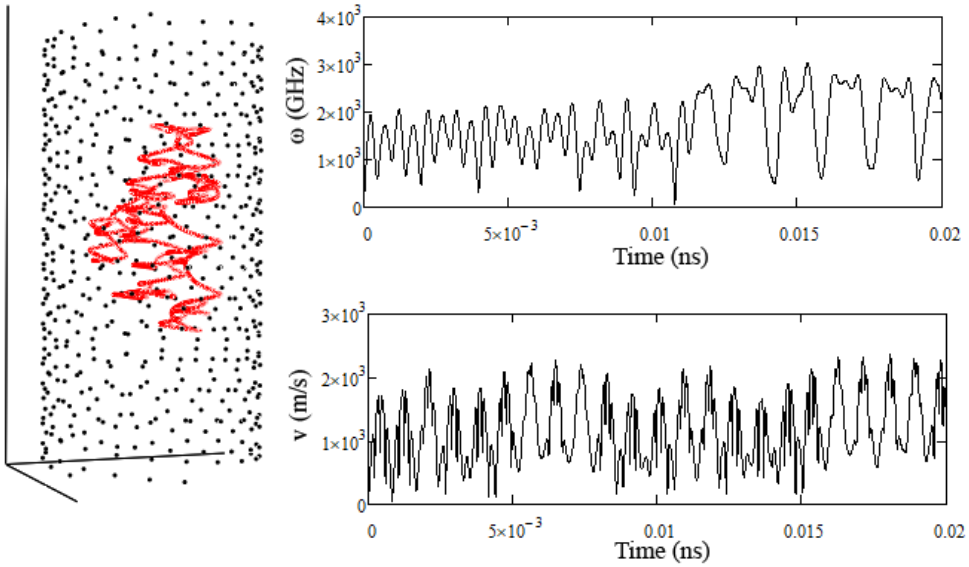

Figure 9. Induced by the electric field and the interatomic interaction forces of rotation C_{60}@CNT(18,2), at a=10 kV/m, f=1000GHz.

All the carbon nanotubes considered in this work were 3 nm long. However, despite this, CNTs had different chiralities, which implies different tube diameters, which can be determined using equation (8). The C_{60}@CNT complexes considered above are given in order of increasing diameter.

$$D = \frac{\sqrt{3}d_0}{\pi}\sqrt{m^2 + n_2 + mn}. \quad (8)$$

In equation (8), m and n are the chirality indices, d_0 is the carbon bond length. Figure 2 shows a carbon tube having the smallest diameter considered. At the initial moment of time, the centers of mass of fullerene and the tube are practically aligned. As calculations of angular oscillations show in this case, almost none. However, there are translational movements of fullerene along the axis of the tube. An applied electric field, whose vector is always in the plane perpendicular to the tube axis, gives fullerene oriented rotations with the angular velocity vector parallel to the tube axis (Fig. 3). In this case, significant transverse vibrations of fullerene arise. As follows from fig. 4, only translational displacements of C_{60} fullerenes are also recorded in a tube of a larger cross section. The superimposed electric field of the same configuration (Fig. 5) creates both rotations and vibrations of fullerene. In a tube with a diameter of 1.43 nm (Fig. 6), natural fullerene rotations appear. Moreover, its natural vibrations are even less intense than in the two previous cases. In the considered example, an external electric field generates intense oriented rotations with slow movement of the fullerene center of mass along the tube axis (Fig. 7). Finally, in the largest tube (Fig. 8, 9), natural rotations appear, having an intensity already lower than in the previous example. Natural vibrations are also less intense. An electric field generates oriented fullerene rotations (Fig. 9).

Acknowledgments

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Исследование состояния C_{60}@CNT в присутствии электрического поля

Димитър Карастоянов[1], Алексей Бубенчиков[2], Михаил Бубенчиков[2] Дмитрий Мамонтов[2] Александр Лун-Фу[3]

[1]Institute of Information and Communication Technologies – BAS

[2]Departamenf of mechanics, Tomsk State University, Tomsk 634050, Russia.

[3]Gazprom transgaz Tomsk, Tomsk 634029, Russia.

Email: orevaore@mail.ru

Аннотация. *В работе представлена математическая модель для численных симуляций вращающихся фуллеренов в углеродных нанотрубках различной хиральности. Проанализированные естественные вращения C_{60}@CNT, а также регулярные и ориентированные вращения, обусловленные действием внешнего гармонически меняющегося во времени электромагнитного поля. Расчеты показывают, что регулярных вращения можно добиться только в случае изначально центрированных C_{60} по отношению к CNT.*

Ключевые слова: *Фуллерен, углеродная нанотрубка, математическое моделирование, молекулярная механика.*