Stable rotation of fullerenes in molecular crystal structures

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Abstract. A large number of various fullerenes and their analogues, each of which individually has different properties, are known. This work presents a consideration of several types of fullerenes in various structures. Using a mathematical model of molecular dynamics we aim to understand the behavioural nature of such structures and answer the questions concerning the reasons for the occurrence of unique properties of individual molecules and crystals, as well as structures consisting of them. We also discuss possible influences on properties of nanomaterials. Finally, we suggest a forecast on how the materials under consideration can be applied.

1. Introduction
Nanomaterials are currently penetrating into various branches, and more and more applications in most important fields of activity are being found: medicine [1], biology [2], electronics [3], materials [4], etc. The greatest demand is for nanomaterials which can be called carbon-based materials - graphenes, fullerenes, carbon nanotubes and their derivatives.

2. Mathematical model
The mathematical model uses the method of molecular dynamics. In all the calculations we use the pair interaction potential — the LJ-potential with parameters given in [5]. To determine orientations of bodies in space we solve the Euler dynamic equations.

2.1. Results and discussion
The calculations were performed for the following structures: standard fullerite with a FCC lattice (temperatures above 260 K) and the onion nanocomplex C_{20}@C_{80}, C_{60}@CNT. For each case, the positions of all atoms at all instants of time were determined under different initial conditions (different orientations of molecules and positions of centres of mass relative to average positions). The effect of electromagnetic fields on fullerenes with an electric charge was also investigated. The calculated rotation velocity of fullerenes in the most studied material, i.e. fullerite, is consistent with the data given in [6], and the energy balance is also observed.
Figure 1a shows a C_{60} fullerene located inside a carbon nanotube, and figure 1b shows the trajectory of one of the fullerene atoms with an electric charge which is placed in a plane rotating electric field whose rotation axis coincides with the axis of the carbon nanotube (16.5). In the case of natural displacements of the fullerene located exactly in the centre of the nanotube (absence of an electric field), the average linear displacement velocity is only 10 m/s, and the rotation frequency is about 7 GHz (figure 2). If the initial position of the fullerene does not coincide with the centre of the nanotube, both the linear and the angular velocities can be 2 orders of magnitude higher. In the presence of an electric field with a strength of 10 kV/m and a frequency of up to 1000 GHz the linear velocity of the fullerene’s centre of mass can move at up to 1000 m/s, and the frequency reaches a value of 1000 GHz. Moreover, even without orientating the fullerene by means of a magnetic field, the C_{60} does not leave the space of the open carbon nanotube.

Figure 2. Rotations of C_{60}@CNT (16.5) in absence of electric field.
Figure 3. C_{20}@C_{80} (a - static state; b - trajectory model of dynamic state).

Figure 3 shows a bimolecular complex. On the left is the static model, on the right is the dynamic model corresponding to the case when the external fullerene is charged and exposed to an external electric field.


![Figure 3](image)

Figure 4. Rotation frequency of fullerene in fullerite.

We also calculated natural rotations and rotations in an electromagnetic field for the case of fullerite. Figure 4 shows the average rotation frequency of a fullerene in fullerite at room temperature $f = 100$ GHz. Under the influence of an electromagnetic field it is possible to create stable rotations of all fullerenes in one direction, as well as to control frequencies of their rotations.

![Figure 4](image)

Figure 5. Ratio of C_{20} rotational velocities to C_{80} rotational velocities in nanocomplex C_{20}@C_{80}.
The calculated velocities of the C$_{20}$ and the C$_{80}$ appeared to be 2700 GHz and 170 GHz for the case of the C$_{20}$@C$_{80}$, i.e. the relation is the same as the inertia moments of the C$_{20}$ and the C$_{80}$, as shown in figure 5.

3. Conclusion
As shown by the calculations, endohedral fullerenes always rotate. Moreover, natural rotations have the nature of angular oscillations followed by a change in the position of the oscillation axis in space. Additionally, the oscillation frequency is determined by the degree of convergence between the fullerene and the shell. In the centered initial state of the system the frequency is usually not very high. However, if a fullerene is ionized, it is possible to initiate regular oriented rotations. In this case, the fullerene frequency is determined by the frequency of the external electric field. In other words, the energy of the external electromagnetic field can be redistributed to the internal degrees of freedom of the material. In such a case, due to the relative independence of vibrations and rotations, the temperature determined by the vibrations of carbon atoms in the systems under consideration does not radically increase. If to consider the complexes C$_{60}$@CNT and C$_{20}$@C$_{80}$ as building blocks for new materials, such materials are able to accumulate a large amount of energy. Oriented rotations prevent compression of a material, i.e. increase its hardness in periodic systems such as bimolecular crystals; the magnetic forces acting between coaxially rotating fullerenes contribute to compaction of the material. Thus, it appears possible to control properties of constructed materials using external electromagnetic fields of a specific configuration.

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