Forced rotation of fullerenes in an electromagnetic fields

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Abstract. A mathematical model of molecular dynamics is presented, which allows one to study the behavior of molecular crystals both in electromagnetic fields and in the absence of fields. This model is universal and affordable, and also does not require high computing power. The fullerene-based materials continue to exhibit unique properties, and the applicability of such materials is steadily increasing. A study of fullerite in the solid phase with charged fullerenes was carried out, characteristic states of the substance were obtained, and their potential properties were analyzed. The potential use of the material is also described taking into account the properties obtained.

1. Introduction

The study of carbon materials, and especially those containing fullerenes in their composition, is of great interest for the development of technologies used in various branches of activity, including medicine. In [1], the vibrational-rotational-translational spectrum of molecular hydrogen in fullerite lattices was considered. [2] demonstrated the impact load of a graphene sheet when exposed to fullerene is theoretically analyzed. [3] showed the mechanical and chemical interactions of defective graphene with large fullerenes are studied C_{240} и C_{540}. In [4], using molecular dynamics, the state of an extremely small cluster consisting of only seven C_{60}. [5] investigated using the Tersoff potential, the vibrational frequencies of each fullerene from the next fullerene family were determined C_{60}, C_{80}, C_{180}, C_{240}, C_{260}, C_{320}, C_{500}, C_{720}. In [6], using the principles of atomistic modeling, the thermal and dynamic characteristics of the onion complex are studied. [7] studied the processes of wrapping fullerenes with graphene sheets were considered. In [8], based on the Tersoff potential for carbon, the anharmonicity of vibrational modes in fullerenes was considered. [9] analysed vibrations of fullerenes in the vicinity of a graphene sheet were considered. [10] considered the magnetic properties of sulfonated fullerene are used. The work [11] is devoted to the synthesis of conjugated triblock derivatives of fullerene. [12] investigated a new hybrid nanocomposite was obtained, including fullerenes for applications in thermoelectronic energy. In [13], fullerenes were functionalized for biomedical applications. [14] described the elastic properties of polymer nanocomposites reinforced with fullerenes and onion structures were considered. [15] demonstrated the magnetization of fullerenes due to the presence of magnetic atoms in them is theoretically considered. [16] determined a new form of the model of a nonlocal spherical shell is formed with reference to the problem of free vibrations of spherical fullerenes. The vibrational analysis of the C_{60} and C_{30} shells was carried out [17] using the nonlinear elastic element method. [18] investigated the design of a new carbon hybrid material consisting of

fullerenes and graphene sheets was presented. Authors [19] described diffusion studies of spherical molecules, in particular, C_{60} fullerenes, were carried out. [20] analysed the development of a new material based on fullerite with ultrahigh stiffness is presented. The rotation of C_{60} in fullerite material was considered in [21]. Fullerenes were discovered in 1985 and have since been thoroughly studied. More than 25,000 scientific articles in English are devoted to Fullerenes because of their wide distribution and unique properties. Fullerenes are ubiquitous in nature. On Earth, they are found in sediments, atmosphere and meteorites [22,23]. In space, fullerenes are also apparently very widespread [24]. In addition to the standard C_{60} fullerenes, there is a whole family of fullerenes consisting of twenty carbon atoms, up to several thousand atoms, and make up completely different materials, standard fullerite, fullerides, sandwich structures, and others. This gives fullerene-based materials a wide range of unique properties, for example, fullerite has very high hardness at low density, under various conditions it can exhibit dielectric properties or superconductivity, have low and high thermal conductivity, have high thermal stability [6], fire resistance and others.

Due to its diversity, the buckyballs family is already widely used in medicine [13], moreover, they have now learned to synthesize water-soluble fullerenes [25], which will give fullerenes even more prospects in medicine. Also, fullerenes are widely used for reinforcing materials and in the energy sector, for example, for the production of solar batteries [11]. This suggests the need to study the spectrum of material properties under various conditions; these materials have great potential to be used in a wide variety of fields. The aim of this work is to demonstrate the ability to generate regular rotations in fullerenes in solid fullerite. In this case, the generated rotations must not violate the crystalline structure of the material. In this case, we can talk about the accumulation of energy on the rotational degrees of freedom of the material, i.e. about increasing internal energy without increasing temperature. High-energy materials have unique mechanical properties that can be predicted through mathematical modeling.

2. Mathematical model

2.1. Model description

In the absence of electromagnetic fields, the frequency of rotation of fullerenes in the solid phase of fullerite, calculated using the following model, coincides with [21,26]. In the current problem, we consider fullerite, in each fullerene of which there are iron atoms with an electric charge, and the magnetic moment is induced due to the rotation of a charged fullerene, perpendicular to the direction of rotation of the charge. An electric charge is on the surface of fullerene and has a charge $q = 9.6 \cdot 10^{-19}$ C. The electric field has an amplitude of E_0=100 kV/m and a frequency f of up to 1000 GHz, and a constant magnetic field of B_0=1 T. In this model, the bond energy and torsion energy are not taken into account, since it is known that no chemical bonds are formed or broken in the fullerite and the fullerenes rotate freely, but the use of bond-oriented potentials will significantly increase the calculation time. For intermolecular interactions, the *LJ*-potential with parameters is used [21]. Oscillations of atoms are simulated in a simplified form, each atom participates in random harmonic vibrations, with a frequency 10^{13} Hz and amplitude of 3-10% of the length of C-C bonds. All calculations were carried out without using existing software packages.

2.2. Forces of cross atom-atom interactions

It is known that the interaction of C_{60} molecules in fullerite is of Van der Waals nature.

The magnitude of the force acting on an individual atom of the C_{60} molecule can be determined if the interaction potential is known: molecule-molecule. In this case, the force will be the gradient of the potential taken with the opposite sign. The potential of intermolecular interaction for fullerenes 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). Thus, the projection of forces:

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

(1)

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

(2)

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

(3)

Here X_k, Y_k, Z_k – are the projections of the all the resulting forces (acting on the k-th atom of the molecule under consideration from other atoms of the crystal) on the axis of the stationary reference system; $r_{kj} = \left|\mathbf{r}_k - \mathbf{r}_j\right|$, $\mathbf{r}_k$ 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 central fullerene atoms, $U(r_{kj})$ – is the potential of the "atom-atom" interaction.

2.3. Rotation of fullerenes in the presence of electromagnetic fields
The dynamic Euler equations for the projections of the angular velocity on the fullerene-fixed axis in this case have the form:

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

(4)

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

(5)

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

(6)

Here the quantities with the index «^{m}» on top 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 axis of the moving reference system; 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.

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

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

(7)

Here M – is the mass of the molecule, 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, is the electric field vector, **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 field.

3. Results of calculations

In all calculations, the magnetic field was constant, and the electric field was harmonically changing and flat. 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. Figures 1-4 (axis dimension is shown in nanometers) show the trajectories of three points, the points located on the fullerene magnetic pole, the equator and the points located between the pole and the equator, marked in red, blue and black, respectively. As can be seen from Figure 1, in the absence of external electromagnetic fields, the regular nature of the rotation of fullerenes is absent. Figure 2 shows the regular rotation mode with the rollover of the fullerene magnetic axis. This occurs at a frequency of 500 GHz. Figure 3 shows the trajectories at a frequency of 50 GHz and in the presence of a sufficiently strong magnetic field. As can be seen from the figure, in this case the trajectories are also regular. Figure 4 shows the mode of stable regular rotation (f=1000 GHz).
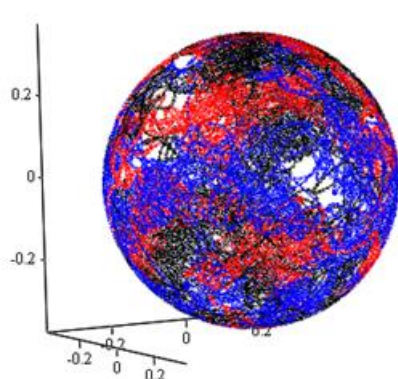

Figure 1. The trajectories of the three points of fullerene in the absence of electromagnetic fields
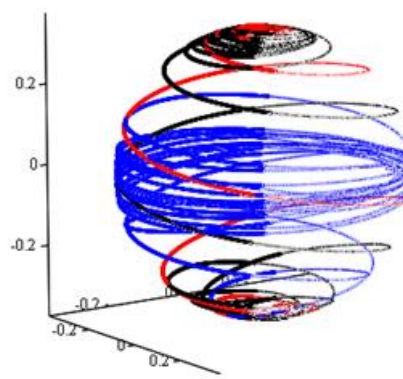
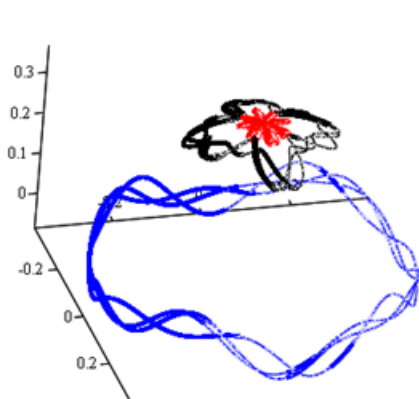**Figure 2.** The trajectories of the three points of fullerene B=1 T, E_0=100 kV/m, f=500 GHz

Figure 3. The trajectories of these same points B= 5 T, E_0=100 kV/m, f=50 GHz
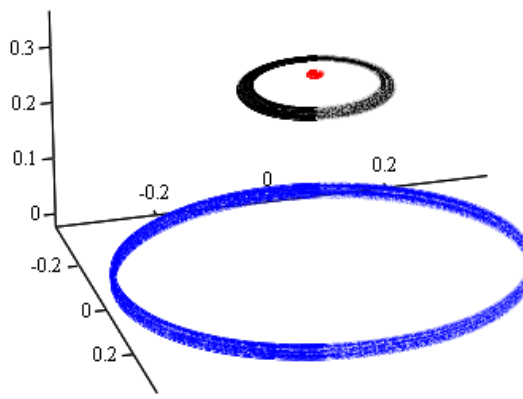
Figure 4. Trajectories of three points on fullerene B=1 T, E_0=100 kV/m, f=1000 GHz

It should be noted that the kinetic energy of regular rotations, as well as the energy of unidirectional translational displacements, should not contribute to the temperature. The latter is usually determined through the energy of chaotic (irregular) displacements. Therefore, the authors consider the promotion of fullerenes by electromagnetic fields as a way of energy storage of material at internal degrees of freedom.

With these parameters, electromagnetic fields are predominant in the rotations of fullerenes, far exceed the forces of intermolecular interactions. Figure 5 shows the change in the frequency of rotation of fullerenes from the frequency of an external electric field. As expected with the configuration of an electromagnetic field capable of involving charged fullerenes (constant magnetic field and plane alternating electric), the angular velocity increases almost linearly with frequency. Calculations showed that the rotation of fullerenes is oriented in one direction. Moreover, in order to achieve characteristic rotations, superstrong fields are not required.
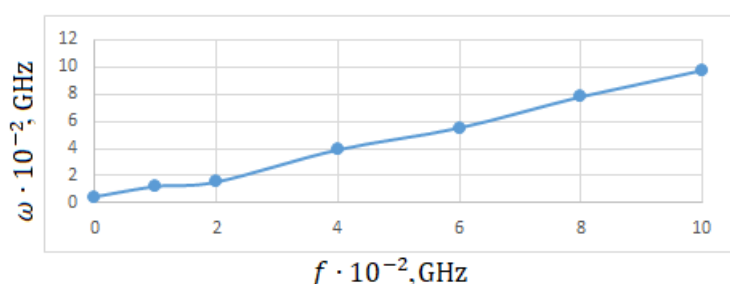

Figure 5. The dependence of the frequency of rotation of fullerenes on the frequency of the external electric field.

4. Conclusion

Oriented directed rotation of fullerenes in the material can be obtained even at weak magnetic fields, for example, to generate a constant magnetic field, it is sufficient to use neodymium magnets. Electric fields can also be weaker than those presented, then the trajectory described by the point on the fullerene equator will take the form not of a circle, but of a wider ring. It is possible to create completely different designs, for example, alternating the charge of fullerenes, which should strengthen the material, while the neighboring fullerenes will rotate in different directions. Since the force of the electromagnetic field acting on fullerenes exceeds the force of their intermolecular interaction, no disturbances in the structure will be caused. The only obstacle to creating such rotation in fullerite will be vacuum. If you try to do this under the conditions of the Earth's atmosphere, the temperature of the rotations and oscillations will come to equilibrium, which means it will be impossible to achieve the presented rotation frequencies.

The speed of rotation directly affects the properties of the material, for example, a rotating fullerene having a charge will generate dipole radiation. Fullerenes rotating at high speed exhibit gyroscopic properties that prevent deformation of the material. This will significantly increase the hardness of the fullerite crystal. However, on the other hand, if the material leaves its stable state, a large amount of heat can be released (the accumulated kinetic energy of rotations which, in the absence of external particles, is not transferred to other groups of movements, but upon impact, most of this stored energy will go to vibrational degrees of freedom), which may also be one of the potential uses of this material.

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