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Numerical Simulation of Interaction between Kr+ Ion and Rotating C₆₀ Fullerene towards for Nanoarchitectonics of Fullerene Materials

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Abstract: Dynamics of charged fullerene in a surface layer of fullerite is studied under the influence of neutral or charged particles of the gas phase surrounding the fullerite material. The translational displacements of the nodes of the crystal lattice structure are determined by the equations of motion of the centers of mass of fullerenes. Central fullerene, which is described as a discrete set of sixty carbon atoms, plays a special role in the presented mathematical model. Angular oscillations and rotations of the central fullerene are described by the dynamic Euler equations. All other fullerenes have a centrally symmetric field of the potential of interaction with the surrounding atoms and molecules. In this regard, we use the hybrid discrete–continuous mathematical model with four potentials that describe the interactions between the surrounding fullerenes, smoothed fullerene and an atom, a pair of atoms, and electric charges. The results of a numerical study of influence of the Coulomb interaction on the rotational and translational motion of the C₆₀ fullerene are presented.

Keywords: molecular crystals; rotating fullerene; incident particle; fullerite; intermolecular interaction; Coulomb interaction

1. Introduction

Since the discovery of C_{60} fullerene in 1985 [1], research is being actively carried out to obtain new fullerene-containing materials. A large number of works on the synthesis of carbon nanomaterials has led to the emergence of nanoarchitectonics [2,3]. According to this universal concept, the fabrication of new functional materials from nanoscale building blocks is achieved through the fusion of nanotechnology with other research disciplines. Today, in synthesis technologies, the decisive role of regulating the functions and properties of nanoscale objects and structures is generally recognized. This makes it possible to produce materials with new properties using the method of self-assembly of molecules [4,5].

Fullerenes can be viewed as simple and fundamental building blocks of a monoelement nature. There are many types of fullerenes, with numbers of carbon atoms up to 980. However, the most stable and common form of fullerene is the C_{60} fullerene, in which six carbon atoms are located on a spherical structure at the vertices of a truncated icosahedron [6]. The C_{60} molecule is easier to manufacture, and therefore widely used. Fullerenes have a number of unique physical, chemical, electrical, and mechanical properties [7–9]. A wide range of materials obtained by synthesis allow us to set tasks for the design of new materials with unique physical properties. These materials are already used in physics research, electronics, and medicine, and have great potential applications in other areas.

Various methods are used to obtain materials based on fullerenes, in particular, the method of interaction of accelerated ions with fullerite films [10–13], laser sputter-



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Copyright: © 2021 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (https:// creativecommons.org/licenses/by/ 4.0/). ing [1,14,15], the electric arc [16,17], gaseous [18-21], and radiation methods [22,23]. Destruction of the fullerite crystal structure can occur in the process of ion implantation with strong fragmentation [24-26] or knocking out individual carbon atoms from the framework of the C_{60} molecule [27]. It is known that, due to the action of intermolecular forces through the weak van der Walls interactions, fullerenes at the nodes of a fullerite crystal behave like high-frequency gigahertz nano-oscillators rotating with average angular speeds of 10¹¹ rad/s [28,29]. It should be noted that, with the help of intense pulsed laser radiation, it is possible to impart additional rotational motion to fullerenes [30,31], but in this case, fullerenes are ionized [32]. The rotation frequency of fullerenes filled with magnetic material can be increased by applying an external magnetic field [33]. An increase in the chaotic rotation of C₆₀ molecules due to the thermal excitation of the rotational degrees of freedom paradoxically provides higher stability of the face-centered cubic structure [34]. The rapid rotation of molecules in fullerite changes their energy electronic states without the presence of a magnetic field [35]. The rotational motion of the C_{60} molecule can be used to reduce the external force due to the redistribution of the load on the group of atoms belonging to the fullerene, as well as due to the gyroscopic effect [36–41], which increases the stability of the entire molecular system. These factors contribute to the suppression of possible fragmentation of the crystal structure and an increase in resistance to external influences on the near-surface layer of the material [42]. The problem of particle penetration through a potential barrier was solved with the integration of the Schrödinger differential equation [43].

In this paper, we study the effect of an incident particle on the dynamics of a rotating C_{60} molecule, which is located at the node of a crystalline fragment of fullerite. This problem is solved using molecular dynamics methods [44–48] based on pairwise interaction potentials and Euler mechanics, which allow describing the rotational and translational motion of particles through independent force and moment interactions. A comparative analysis is carried out depending on the charge, speed of the incident particle, and rotational speed of fullerene.

2. Physical Statement of the Problem

We consider the effect of an ionized particle (Kr+, 83.8 a.m.) moving towards the central C_{60} molecule at a speed of 500–2000 m/s (see Figure 1). The central fullerene is composed of sixty carbon atoms. The dynamic state of this fullerene is determined by the nature of the interaction of its atoms with all the surrounding elements of the system. The group of these elements includes, in particular, 12 fullerenes, which, at the initial moment of time, are at a distance of 1.002 nm from the center of mass of the rotating C_{60} molecule. Together, they form the minimum fragment of a face-centered cubic crystal lattice (see Figure 1). The group of elements surrounding the central fullerene also includes the krypton cation. The interaction of an ionized krypton atom with carbon atoms of the central fullerene and surrounding fullerenes is described using the interatomic interaction potentials and Coulomb's law. At the initial moment of time, the central molecule was given an angular velocity in the range from 0 to 2000 rad/ns. Note that the de Broglie wavelengths for a moving particle and fullerene molecule will be noticeably smaller than the diameter of a carbon atom in this case. This makes it possible to use the methods of classical molecular physics to solve this problem, which are widely used to study the dynamic properties of nanoscale materials [44–48]. In this article, we do not take into account the influence of intramolecular vibrational modes, as in our early work [49].



Figure 1. Schema of fullerite consisting of 13 C_{60} molecules. The green sphere refers to a krypton atom.

3. Mathematical Statement of the Problem

We place the global Cartesian coordinate system (*xyz*) in the initial symmetric position of the center of mass of the inner fullerene. The local Cartesian coordinate system ($\xi\eta\zeta$) is associated with the moving fullerene and its oscillating center of mass *C*.

The interaction of a specific carbon atom with the neutral part of the particle will be determined using the attraction–repulsion potential 6–12 of the model of pair interaction of non-polar particles [47,50].

$$U(r_{pk}) = 4\varepsilon \left[\left(\frac{\sigma}{r_{pk}} \right)^{12} - \left(\frac{\sigma}{r_{pk}} \right)^6 \right],$$
(1)

where r_{pk} is the distance between the center of the incident particle and the *k*th carbon atom of central fullerene.

The charge of the incident particle acts on the charge of the central fullerene with the Coulomb force:

$$F_{pC} = k \frac{q_p q_C}{r_{pC}^2} \frac{r_{pC}}{r_{pC}}, \ F_{Cp} = -F_{pC}, \tag{2}$$

where r_{pC} is the vector directed from the center of the incident particle to the center of the fullerene charge q_C ; and k is coefficient of proportionality.

The interaction between surrounding fullerenes is based on the potential proposed by L.A. Girifalco [51]:

$$G(\rho_{ij}) = \alpha \left[\frac{1}{\rho_{ij}(\rho_{ij}-1)^3} + \frac{1}{\rho_{ij}(\rho_{ij}+1)^3} - \frac{2}{\rho_{ij}^4} \right] + \beta \left[\frac{1}{\rho_{ij}(\rho_{ij}-1)^9} + \frac{1}{\rho_{ij}(\rho_{ij}+1)^9} - \frac{2}{\rho_{ij}^{10}} \right],$$
(3)

where $\rho_{ij} = r_{ij}/2a$, r_{ij} is the distance between the centers of the *i*th and *j*th molecules of the smoothed C₆₀; $\alpha = 74.94 \times 10^{-15}$ erg; and $\beta = 135.95 \times 10^{-18}$ erg.

Neutral surrounding fullerenes have a centrally symmetric potential of interaction with carbon atoms of the central C_{60} and the neutral part of a charged particle [52]

$$\Phi(r_{ik}) = \frac{4\varepsilon a\pi}{r_{ik}A} \left[\frac{\sigma^{12}}{5} \left((r_{ik} - a)^{-10} - (r_{ik} + a)^{-10} \right) - \frac{\sigma^6}{2} \left((r_{ik} - a)^{-4} - (r_{ik} + a)^{-4} \right) \right]$$
(4)

where *A* is the area per carbon atom; *a* is the fullerene radius; and r_{ik} is the distance between the center of the *i*th adjacent fullerene and the *k*th carbon atom of the central C₆₀ molecule, $i = \overline{1, 12}$, $k = \overline{1, 60}$. The potential (4) is based on the potential (1), assuming a uniform distribution of potential energy over the area of the sphere. This approach makes it possible to exclude high-frequency oscillations from the solution and to simplify its frequency analysis of the behavior of fullerenes.

The dynamic Euler equations are used to describe the rotational motion of the central fullerene molecule around its own center of mass [46,47]:

$$J_1 \frac{d\omega_{\xi}}{dt} + (J_3 - J_2)\omega_{\eta}\omega_{\zeta} = M_{\xi}^{(e)},\tag{5}$$

$$J_2 \frac{d\omega_\eta}{dt} + (J_1 - J_2)\omega_\zeta \omega_\xi = M_\eta^{(e)},\tag{6}$$

$$J_3 \frac{d\omega_{\zeta}}{dt} + (J_2 - J_1)\omega_{\zeta}\omega_{\eta} = M_{\zeta}^{(e)}.$$
(7)

where ω_{ξ} , $\omega_{\eta} \omega_{\zeta}$ are components of the angular velocity about principal axes; J_1 , J_2 , J_3 are the principal moments of inertia of the molecule for its center of mass; and $M_{\xi}^{(e)}$, $M_{\eta}^{(e)}$, and $M_{\zeta}^{(e)}$ are the projections of the moments of forces on the ξ , η and ζ -axis.

Equations (4)–(6) are closed by Euler's kinematic relations, connecting the components of the angular velocity with the Euler angles φ , ψ , θ :

$$\omega_{\xi} = \psi \sin \theta \sin \phi + \theta \cos \phi, \qquad (8)$$

$$\omega_{\eta} = \psi \sin \theta \cos \phi - \theta \sin \phi, \tag{9}$$

$$\omega_{\zeta} = \psi \cos \phi + \phi, \tag{10}$$

where the dot is used to signify time derivatives.

Thus, two simple crystallographic models are used to describe fullerenes: a central fullerene with icosahedral symmetry and spherical surrounding uncharged fullerenes. Therefore, translational displacements of the surrounding fullerenes will be determined by the following equations:

$$M\frac{d\boldsymbol{v}_f}{dt} = \sum_{k=1}^{N-1} \nabla G\left(r_{fk}\right) + \sum_{k=1}^{S} \nabla \Phi\left(r_{fk}\right), \ \boldsymbol{v}_f = \frac{d\boldsymbol{r}_f}{dt}.$$
 (11)

The dynamic state of the central fullerene is determined by the nature of the interaction of sixty carbon atoms with all elements of surroundings. Therefore, the motion of the center of mass of the central fullerene obeys the following law:

$$M\frac{dv_{c}}{dt} = \sum_{k=1}^{N} \sum_{i=1}^{S} \nabla \Phi(r_{ik}) + \sum_{i=1}^{S} \nabla U(r_{pi}) + F_{pC}, \ v_{C} = \frac{dr_{C}}{dt}.$$
 (12)

The motion of the center of mass of a charged particle obeys the equation

$$m_p \frac{dv_p}{dt} = \sum_{i=1}^{N} \nabla \Phi(r_{pi}) + \sum_{k=1}^{S} \nabla U(r_{pk}) - F_{pC}, \ v_p = \frac{dr_p}{dt}.$$
(13)

In Equations (11)–(13), M is the fullerene mass; m_p is the particle mass; ∇ is gradient operator; S = 60 is the number of carbon atoms in the C_{60} molecule; N = 12 is the number of surrounding fullerenes; r_{fk} is the distance between the center of the considered smoothed fullerene and the center of the kth carbon atom on the inner fullerene; r_{pk} is the distance from the center of the particle to the center of the kth carbon atom on the center of the central fullerene; r_{pi} is the distance from the center of the particle to the center of the ith surrounding fullerene; G is the potential of L.A. Girifalco [51]; and the subscripts p, C, and f refer to the particle, the central polyatomic fullerene, and the center of the smoothed fullerene, respectively.

The initial conditions for solving the system of differential Equations (5)–(13) are given in the following form:

$$t = 0: \ \psi = \psi^0, \ \theta = \theta^0, \ \phi = \phi^0, \ \omega_{\xi} = \omega_{\xi}^0, \ \omega_{\eta} = \omega_{\eta}^0, \ \omega_{\zeta} = \omega_{\zeta}^0, \tag{14}$$

$$v_{C} = 0, r_{C} = 0, v_{f} = 0, r_{f} = r_{f}^{0}, v_{p} = v_{p}^{0}, r_{p} = r_{p}^{0}.$$
 (15)

We apply a fourth-order accurate scheme [53] using the idea of recalculating the sought quantities within a separate time step to solve the system of Equations (5)–(13) with initial conditions (14) and (15). This allows us to determine the dynamic characteristics of the incident charged particles and each atom of the central fullerene.

4. Results and Discussion

Consider the C_{60} fullerene, which is at rest at the initial moment of time. It has a charge $q_f = 1$ e and an angular velocity $\omega^0 = 0$ rad/s (see Figure 1). The x and ζ -axes coincide at the initial moment of time. Thus, the Euler angles ψ , θ (8)–(10) will determine the orientation of the ζ -axis in space. At this moment, the incident particle (Kr+, 83.8 a.m.) is in position (-4, 0, 0) and has a charge $q_p = 1$ e or $q_p = 0$. In the calculations, the initial velocity of the incident particle varied from 500 to 2000 m/s.

Figure 2 shows the trajectory of the incident particle as function x(t). As can be seen from the figure, the neutral particle (solid curves) approaches the central fullerene rather closely (0.65 ± 0.02 nm) for all the considered values of its initial velocity. However, the position of the deceleration zone strongly depends on its velocity in the case of a charged particle (dashed curves). At a speed of $v_p = 500$ m/s, a charged particle under the action of Coulomb forces completely loses its speed at a sufficiently large distance (x = -2.9 nm) and then begins to move in the opposite direction. At $v_p = 1000$ m/s for a charged particle, this occurs at x = -1.45 nm. At 2000 m/s, the effect of the charge has little effect on the nature of the particle motion.

Let us consider the central fullerene. Figure 3 illustrates the time dependence of the *x*-coordinate of the central of the central fullerene. The *y*- and *z*-coordinates are not shown, since they change slightly. Figure 3 illustrates the damping effect of the Coulomb interaction. It is seen that the presence of a charge significantly reduces the effect of the test particle on the central fullerene. An almost complete shielding of the force action of charged particle occurs at initial velocity up to 1000 m/s. At $v_p = 2000$ m/s, the presence of a charge reduces the deviation of the central fullerene from the initial position by 30.8%.

The action of a charged or neutral particle leads to a change in the rotational dynamics of the central fullerene. In the absence of a particle, the angular velocity of rotation of the inner fullerene varies from 0 to 670 rad/ns. These results are in qualitative agreement with the experimental data obtained using spectrographic measurements [28,29,54], according to which the angular speed is the order of 10^2 rad/ns. At $v_p = 1000$ m/s, the amplitude of the angular velocity increases by 8.9% after the action of the neutral particle (Figure 4). However, the impact of a charged particle did not affect the magnitude of the angular velocity. The change in the amplitude of the angular velocity is caused by the resulting force, which is not parallel to the axis of rotation and changes its direction due to the rotation of carbon atoms. This causes the appearance of an external torque, which increases the angular momentum of the rotating fullerene. Thus, the external force acting on the fullerene molecule leads to a change in the rotational motion.



Figure 2. The ion and neutral particle trajectories.



Figure 3. Trajectory of the center of mass of the internal C_{60} molecule at $\omega^0 = 0$ rad/s.



Figure 4. Time dependence of the instantaneous angular velocity component ω_x ($v_p = 1000 \text{ m/s}$).

As can be seen from Figure 4, the fullerene changes the direction of its rotation. This means that the central fullerene performs angular oscillations, which are primarily due to the influence of the surrounding C₆₀. To overcome the influence causing angular oscillations, fullerene must be given the initial angular rotation velocity $\omega^0 > 1000 \text{ rad/ns}$ (see Figure 5). As can be seen from this figure, a stable rotational motion is observed at $\omega^0 > 1000$ in the direction along the angle θ in the absence of rotation in other angular directions.



Figure 5. Time dependence of the intrinsic rotation angle θ for different initial rotation rate of fullerene.

Figure 6a shows that an incident neutral particle with a velocity of $v_p = 1000 \text{ m/s}$ increases the maximum rotation speed of the C₆₀ fullerene by 1.8% and 3.6% for $\omega^0 = 1500$ and 2000 rad/ns, respectively. The charged particle had no effect on the angular velocity.



Figure 6. Time dependence of instantaneous angular velocity: (a) $v_p = 1000 \text{ m/s}$, (b) $v_p = 2000 \text{ m/s}$.

At $v_p = 2000$ m/s, a neutral particle increases the maximum rotation speed of fullerene by 11.5% and 4.8%, and a charged particle increases it by 4.7% and 1.1% for $\omega^0 = 1500$ and 2000 rad/ns, respectively (see Figure 6b). It is seen that a charged particle has a weaker effect on the fullerene rotation dynamics. Note that the growth of the amplitude mainly depends on the value of v_p , as well as on the dynamic state of the fullerene.

As can be seen from Figure 7, the presence of a charge on a particle leads to a smaller shift of the fullerene center of mass relative to its initial position (22.6–23.6 pm) than in the absence of a charge (31.7–35.3 pm). However, the trajectories of the neutral and ionized particles differ little from each other at $v_p = 2000$ m/s (Figure 2). Consequently, the Coulomb force (Equations (12) and (13)) reduces the effect of an incident particle on the translational and rotational dynamics of the C₆₀ fullerene. It should be noted that the damping effect is enhanced by the action of bivalent and trivalent cations on the rotating fullerene. Along with this, the force effect will be less pronounced for higher fullerenes (C₇₀, C₇₈, etc.) due to their greater mass compared to the C₆₀ fullerene.



Figure 7. Trajectory of the center of mass of the internal C_{60} molecule at $v_p = 2000$ m/s.

5. Conclusions

In this article, we have presented the hybrid discrete–continuous mathematical model of the interaction between a krypton ion and the C_{60} fullerene in crystalline fullerite. The molecular dynamics study of the force effect of an incident atom on a rotating fullerene molecule has been carried out. Analysis of the calculation results shows that fullerene retains a more stable position when the incoming particle has a charge. An almost complete shielding of the force action is observed for incident charged particles with a low speed of movement up to 1000 m/s. The amplitude of the angular velocity of fullerene increases more strongly under the impact of an incident neutral particle than under a charged particle. The C_{60} fullerene in a fullerite crystal is able to obtain additional angular acceleration under the action of an external force. The calculation results show that the rotational dynamics of C_{60} fullerene can be controlled by choosing the velocity and charge of the incident particles. This makes it possible to change the characteristics of both the initial fullerene material and the synthesized materials.

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References

- 1. Kroto, H.W.; Heath, J.R.; O'Brien, S.C.; Curl, R.F.; Smalley, R.E. C₆₀: Buckminsterfullerene. Nature 1985, 318, 162–163. [CrossRef]
- 2. Ariga, K. Nanoarchitectonics: What's Coming next after Nanotechnology? Nanoscale Horiz. 2021, 6, 364–378. [CrossRef]
- 3. Maji, S.; Shrestha, L.K.; Ariga, K. Nanoarchitectonics for Hierarchical Fullerene Nanomaterials. *Nanomaterials* **2021**, *11*, 2146. [CrossRef]
- 4. Neal, E.A.; Nakanishi, T. Alkyl-Fullerene Materials of Tunable Morphology and Function. *Bull. Chem. Soc. Jpn.* **2021**, *94*, 1769–1788. [CrossRef]
- Maji, S.; Shrestha, R.G.; Lee, J.; Han, S.A.; Hill, J.P.; Kim, J.H.; Ariga, K.; Shrestha, L.K. Macaroni Fullerene Crystals-Derived Mesoporous Carbon Tubes as a High Rate Performance Supercapacitor Electrode Material. *Bull. Chem. Soc. Jpn.* 2021, 94, 1502–1509. [CrossRef]
- 6. Terrones, H.; Terrones, M. Curved Nanostructured Materials. *New J. Phys.* 2003, *5*, 126. [CrossRef]
- 7. Goodarzi, S.; Da Ros, T.; Conde, J.; Sefat, F.; Mozafari, M. Fullerene: Biomedical Engineers Get to Revisit an Old Friend. *Mater. Today* **2017**, *20*, 460–480. [CrossRef]
- 8. Veclani, D.; Tolazzi, M.; Melchior, A. Molecular Interpretation of Pharmaceuticals' Adsorption on Carbon Nanomaterials: Theory Meets Experiments. *Processes* **2020**, *8*, 642. [CrossRef]
- 9. Wilson, M.A.; Pang, L.S.K.; Willett, G.D.; Fisher, K.J.; Dance, I.G. Fullerenes—Preparation, Properties, and Carbon Chemistry. *Carbon* **1992**, *30*, 675–693. [CrossRef]
- 10. Neyts, E.; Maeyens, A.; Pourtois, G.; Bogaerts, A. A Density-Functional Theory Simulation of the Formation of Ni-Doped Fullerenes by Ion Implantation. *Carbon* **2011**, *49*, 1013–1017. [CrossRef]
- Makarets, M.V.; Prylutskyy, Y.I.; Ogloblya, O.V.; Carta-Abelmann, L.; Scharff, P. Computer Simulation of Supported C₆₀ Fullerenes Fragmentation by Particle Beam. *Carbon* 2004, *42*, 987–990. [CrossRef]
- 12. Tellgmann, R.; Krawez, N.; Lin, S.-H.; Hertel, I.V.; Campbell, E.E.B. Endohedral Fullerene Production. *Nature* **1996**, *382*, 407–408. [CrossRef]
- Pietzak, B.; Waiblinger, M.; Murphy, T.A.; Weidinger, A.; Höhne, M.; Dietel, E.; Hirsch, A. Buckminsterfullerene C₆₀: A Chemical Faraday Cage for Atomic Nitrogen. *Chem. Phys. Lett.* **1997**, 279, 259–263. [CrossRef]
- 14. Heath, J.R.; O'Brien, S.C.; Zhang, Q.; Liu, Y.; Curl, R.F.; Tittel, F.K.; Smalley, R.E. Lanthanum Complexes of Spheroidal Carbon Shells. J. Am. Chem. Soc. 1985, 107, 7779–7780. [CrossRef]
- 15. Guo, T.; Diener, M.D.; Chai, Y.; Alford, M.J.; Haufler, R.E.; McClure, S.M.; Ohno, T.; Weaver, J.H.; Scuseria, G.E.; Smalley, R.E. Uranium Stabilization of C28: A Tetravalent Fullerene. *Science* **1992**, 257, 1661–1664. [CrossRef]
- Krätschmer, W.; Lamb, L.D.; Fostiropoulos, K.; Huffman, D.R. Solid C₆₀: A New Form of Carbon. *Nature* 1990, 347, 354–358.
 [CrossRef]
- 17. Lebedkin, S.; Renker, B.; Heid, R.; Schober, H.; Rietschel, H. A Spectroscopic Study of M@C82 Metallofullerenes: Raman, Far-Infrared, and Neutron Scattering Results. *Appl. Phys. Mater. Sci. Process.* **1998**, *66*, 273–280. [CrossRef]
- 18. Saunders, M.; Jimenez-Vazquez, H.A.; Cross, R.J.; Mroczkowski, S.; Gross, M.L.; Giblin, D.E.; Poreda, R.J. Incorporation of Helium, Neon, Argon, Krypton, and Xenon into Fullerenes Using High Pressure. *J. Am. Chem. Soc.* **1994**, *116*, 2193–2194. [CrossRef]
- 19. Saunders, M.; Cross, R.J.; Jimenez-Vazquez, H.A.; Shimshi, R.; Khong, A. Noble Gas Atoms Inside Fullerenes. *Science* **1996**, 271, 1693–1697. [CrossRef]
- DiCamillo, B.A.; Hettich, R.L.; Guiochon, G.; Compton, R.N.; Saunders, M.; Jiménez-Vázquez, H.A.; Khong, A.; Cross, R.J. Enrichment and Characterization of a Noble Gas Fullerene: Ar@C₆₀. J. Phys. Chem. **1996**, 100, 9197–9201. [CrossRef]
- Brink, C.; Hvelplund, P.; Shen, H.; Jiménez-Vázquez, H.A.; Cross, R.J.; Saunders, M. Collisional Fragmentation of Ar@C₆₀. *Chem. Phys. Lett.* **1998**, 286, 28–34. [CrossRef]
- 22. Ohtsuki, T.; Ohno, K.; Shiga, K.; Kawazoe, Y.; Maruyama, Y.; Masumoto, K. Insertion of Xe and Kr Atoms into C₆₀ and C₇₀ Fullerenes and the Formation of Dimers. *Phys. Rev. Lett.* **1998**, *81*, 967–970. [CrossRef]
- 23. Gadd, G.E.; Evans, P.J.; Hurwood, D.J.; Morgan, P.L.; Moricca, S.; Webb, N.; Holmes, J.; McOrist, G.; Wall, T.; Blackford, M.; et al. Endohedral Fullerene Formation through Prompt Gamma Recoil. *Chem. Phys. Lett.* **1997**, 270, 108–114. [CrossRef]
- 24. Tripathi, A.; Kumar, A.; Singh, F.; Kabiraj, D.; Avasthi, D.K.; Pivin, J.C. Ion Irradiation Induced Surface Modification Studies of Polymers Using SPM. *Nucl. Instrum. Methods Phys. Res. Sect. B Beam Interact. Mater. At.* **2005**, 236, 186–194. [CrossRef]
- Narayanan, K.L.; Kojima, N.; Yamaguchi, K.; Ishikawa, N.; Yamaguchi, M. Arsenic Ion Implantation Induced Structural Effects in C₆₀ Films. J. Mater. Sci. 1999, 34, 5227–5231. [CrossRef]
- 26. Todorović-Marković, B.; Draganić, I.; Vasiljević-Radović, D.; Romčević, N.; Blanuša, J.; Dramićanin, M.; Marković, Z. Structural Modification of Fullerene Thin Films by Highly Charged Iron Ions. *Appl. Phys. A* **2007**, *89*, 749–754. [CrossRef]

- 27. Zawislak, F.C.; Baptista, D.L.; Behar, M.; Fink, D.; Grande, P.L.; da Jornada, J.A.H. Damage of Ion Irradiated C₆₀ Films. *Nucl. Instrum. Methods Phys. Res. Sect. B Beam Interact. Mater. At.* **1999**, 149, 336–342. [CrossRef]
- Johnson, R.D.; Yannoni, C.S.; Vries, M.S. de C₆₀ Solid State Rotational Dynamics and Production and EPR Spectroscopy of Fullerenes Containing Metal Atoms. *Nanotechnology* 1992, *3*, 164–166. [CrossRef]
- 29. Johnson, R.D.; Yannoni, C.S.; Dorn, H.C.; Salem, J.R.; Bethune, D.S. C₆₀ Rotation in the Solid State: Dynamics of a Faceted Spherical Top. *Science* **1992**, *255*, 1235–1238. [CrossRef] [PubMed]
- Yang, S.; Wei, T.; Scheurell, K.; Kemnitz, E.; Troyanov, S.I. Chlorination-Promoted Skeletal-Cage Transformations of C₈₈ Fullerene by C₂ Losses and a C–C Bond Rotation. *Chem.-Eur. J.* 2015, *21*, 15138–15141. [CrossRef]
- 31. Meletov, K.P. The Photopolymerization Rate and Activation Energy of C₆₀ Rotations in Fullerene and Its Molecular Complexes. *Fuller. Nanotub. Carbon Nanostruct.* **2020**, *28*, 93–96. [CrossRef]
- 32. Jaroń-Becker, A.; Becker, A.; Faisal, F.H.M. Saturated Ionization of Fullerenes in Intense Laser Fields. *Phys. Rev. Lett.* 2006, 96, 143006. [CrossRef] [PubMed]
- 33. Wolski, P.; Nieszporek, K.; Panczyk, T. Multimodal, PH Sensitive, and Magnetically Assisted Carrier of Doxorubicin Designed and Analyzed by Means of Computer Simulations. *Langmuir* **2018**, *34*, 2543–2550. [CrossRef] [PubMed]
- 34. Raransky, M.D.; Balazyuk, V.N.; Gunko, M.M.; Struk, A.Y. Analysis of Specific Auxetic Properties of Fullerite C60. *East.-Eur. J. Enterp. Technol.* **2015**, *5*, 18. [CrossRef]
- 35. Lima, J.R.F.; Brandão, J.; Cunha, M.M.; Moraes, F. Effects of Rotation in the Energy Spectrum of C₆₀. *Eur. Phys. J. D* 2014, *68*, 94. [CrossRef]
- Passaro, V.M.N.; Cuccovillo, A.; Vaiani, L.; De Carlo, M.; Campanella, C.E. Gyroscope Technology and Applications: A Review in the Industrial Perspective. *Sensors* 2017, 17, 2284. [CrossRef] [PubMed]
- 37. Usubamatov, R. Theory of Gyroscopic Effects for Rotating Objects: Gyroscopic Effects and Applications; Springer: Singapore, 2020; ISBN 9789811564741.
- 38. Gray, R.C. Gyroscopic Principles and Applications. Nature 1944, 153, 277–278. [CrossRef]
- Song, L.; Ci, L.J.; Sun, L.F.; Jin, C.; Liu, L.; Ma, W.; Liu, D.; Zhao, X.; Luo, S.; Zhang, Z.; et al. Large-Scale Synthesis of Rings of Bundled Single-Walled Carbon Nanotubes by Floating Chemical Vapor Deposition. *Adv. Mater.* 2006, 18, 1817–1821. [CrossRef]
- 40. Chao, D.; Jun, H.; Mingyu, T.; Deyang, Z.; Leyong, W. Design, Synthesis and Assembly of Gyroscope-like Molecules. *Prog. Chem.* **2010**, *22*, 1021–1034.
- Lang, G.M.; Shima, T.; Wang, L.; Cluff, K.J.; Skopek, K.; Hampel, F.; Blümel, J.; Gladysz, J.A. Gyroscope-Like Complexes Based on Dibridgehead Diphosphine Cages That Are Accessed by Three-Fold Intramolecular Ring Closing Metatheses and Encase Fe(CO)₃, Fe(CO)₂(NO)⁺, and Fe(CO)₃(H)⁺ Rotators. *J. Am. Chem. Soc.* 2016, 138, 7649–7663. [CrossRef]
- 42. Dmitriev, A.I.; Nikonov, A.Y.; Filippov, A.E.; Psakhie, S.G. Molecular Dynamics Study of the Evolution of Rotational Atomic Displacements in a Crystal Subjected to Shear Deformation. *Phys. Mesomech.* **2019**, *22*, 375–381. [CrossRef]
- 43. Bubenchikov, A.M.; Bubenchikov, M.A.; Potekaev, A.I.; Libin, E.Y.; Khudobina, Y.P.; Kulagina, V.V. Penetration of Microparticles Through Composite Potential Barriers. *Russ. Phys. J.* 2017, *60*, 140–148. [CrossRef]
- 44. Jeong, B.-W.; Kim, H.-Y. Molecular Dynamics Simulations of the Failure Behaviors of Closed Carbon Nanotubes Fully Filled with C₆₀ Fullerenes. *Comput. Mater. Sci.* 2013, 77, 7–12. [CrossRef]
- 45. Kang, J.W.; Hwang, H.J. Molecular Dynamics Study on Oscillation Dynamics of a C₆₀ Fullerene Encapsulated in a Vibrating Carbon-Nanotube-Resonator. *Comput. Mater. Sci.* **2010**, *50*, 790–795. [CrossRef]
- 46. Bubenchikov, A.M.; Bubenchikov, M.A.; Lun-Fu, A.V.; Ovchinnikov, V.A. Gyroscopic Effects in Fullerite Crystal upon Deformation. *Eur. Phys. J. Plus* **2021**, *136*, 388. [CrossRef]
- 47. Bubenchikov, M.A.; Bubenchikov, A.M.; Lun-Fu, A.V.; Ovchinnikov, V.A. Rotational Dynamics of Fullerenes in the Molecular Crystal of Fullerite. *Phys. Status Solidi A* 2021, *218*, 2000174. [CrossRef]
- 48. Piatek, A.; Dawid, A.; Gburski, Z. The Existence of a Plastic Phase and a Solid–Liquid Dynamical Bistability Region in Small Fullerene Cluster (C₆₀)₇: Molecular Dynamics Simulation. *J. Phys. Condens. Matter* **2006**, *18*, 8471–8480. [CrossRef] [PubMed]
- 49. Bubenchikov, A.M.; Bubenchikov, M.A.; Mamontov, D.V.; Kaparulin, D.S.; Lun-Fu, A.V. Dynamic State of Columnar Structures Formed on the Basis of Carbon Nanotori. *Fuller. Nanotub. Carbon Nanostruct.* **2021**, *29*, 825–831. [CrossRef]
- 50. McLure, I.A.; Ramos, J.E.; del Río, F. Accurate Effective Potentials and Virial Coefficients in Real Fluids. 1. Pure Noble Gases and Their Mixtures. J. Phys. Chem. B **1999**, 103, 7019–7030. [CrossRef]
- 51. Girifalco, L.A. Extended Mie-Grüneisen Theory Applied to C₆₀ in the Disordered Fcc Phase. *Phys. Rev. B* **1995**, *52*, 9910–9916. [CrossRef] [PubMed]
- 52. Rudyak, V.Y.A. Statistical Aerohydromechanics of Homogeneous and Heterogeneous Media; NSUACE: Novosibirsk, Russia, 2004; Volume 1, ISBN 5-7795-0228-5.
- 53. Ortega, J.M.; Poole, W.G. An Introduction to Numerical Methods for Differential Equations; Pitman: Marshfield, WI, USA, 1981; ISBN 978-0-273-01686-1.
- Neumann, D.A.; Copley, J.R.D.; Cappelletti, R.L.; Kamitakahara, W.A.; Lindstrom, R.M.; Creegan, K.M.; Cox, D.M.; Romanow, W.J.; Coustel, N.; McCauley, J.P.; et al. Coherent Quasielastic Neutron Scattering Study of the Rotational Dynamics of C₆₀ in the Orientationally Disordered Phase. *Phys. Rev. Lett.* **1991**, *67*, 3808–3811. [CrossRef] [PubMed]