# Numerical Simulation of Interaction between $\mathrm{Kr}+$ Ion and Rotating $\mathrm{C}_{60}$ 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 $\mathrm{C}_{60}$ fullerene are presented.


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

## 1. Introduction

Since the discovery of $\mathrm{C}_{60}$ 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 $\mathrm{C}_{60}$ fullerene, in which six carbon atoms are located on a spherical structure at the vertices of a truncated icosahedron [6]. The $\mathrm{C}_{60}$ 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-
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 $\mathrm{C}_{60}$ 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 $10^{11} \mathrm{rad} / \mathrm{s}[28,29]$. 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 $\mathrm{C}_{60}$ 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 $\mathrm{C}_{60}$ 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 $\mathrm{C}_{60}$ 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 ( $\mathrm{Kr}+, 83.8$ a.m.) moving towards the central $\mathrm{C}_{60}$ molecule at a speed of $500-2000 \mathrm{~m} / \mathrm{s}$ (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 $\mathrm{C}_{60}$ 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 $2000 \mathrm{rad} / \mathrm{ns}$. 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 $13 \mathrm{C}_{60}$ molecules. The green sphere refers to a krypton atom.

## 3. Mathematical Statement of the Problem

We place the global Cartesian coordinate system $(x y z)$ 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].

$$
\begin{equation*}
\mathrm{U}\left(r_{p k}\right)=4 \varepsilon\left[\left(\frac{\sigma}{r_{p k}}\right)^{12}-\left(\frac{\sigma}{r_{p k}}\right)^{6}\right] \tag{1}
\end{equation*}
$$

where $r_{p k}$ 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:

$$
\begin{equation*}
\boldsymbol{F}_{p C}=k \frac{q_{p} q_{C}}{r_{p C}^{2}} \frac{\boldsymbol{r}_{p C}}{r_{p C}}, \boldsymbol{F}_{C p}=-\boldsymbol{F}_{p C}, \tag{2}
\end{equation*}
$$

where $\boldsymbol{r}_{p C}$ 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]:
$G\left(\rho_{i j}\right)=\alpha\left[\frac{1}{\rho_{i j}\left(\rho_{i j}-1\right)^{3}}+\frac{1}{\rho_{i j}\left(\rho_{i j}+1\right)^{3}}-\frac{2}{\rho_{i j}^{4}}\right]+\beta\left[\frac{1}{\rho_{i j}\left(\rho_{i j}-1\right)^{9}}+\frac{1}{\rho_{i j}\left(\rho_{i j}+1\right)^{9}}-\frac{2}{\rho_{i j}^{10}}\right]$,
where $\rho_{i j}=r_{i j} / 2 a, r_{i j}$ is the distance between the centers of the $i$ th and $j$ th molecules of the smoothed $\mathrm{C}_{60} ; \alpha=74.94 \times 10^{-15} \mathrm{erg} ;$ and $\beta=135.95 \times 10^{-18} \mathrm{erg}$.

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

$$
\begin{equation*}
\Phi\left(r_{i k}\right)=\frac{4 \varepsilon a \pi}{r_{i k} A}\left[\frac{\sigma^{12}}{5}\left(\left(r_{i k}-a\right)^{-10}-\left(r_{i k}+a\right)^{-10}\right)-\frac{\sigma^{6}}{2}\left(\left(r_{i k}-a\right)^{-4}-\left(r_{i k}+a\right)^{-4}\right)\right] \tag{4}
\end{equation*}
$$

where $A$ is the area per carbon atom; $a$ is the fullerene radius; and $r_{i k}$ is the distance between the center of the $i$ th adjacent fullerene and the $k$ th carbon atom of the central $\mathrm{C}_{60}$ 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]:

$$
\begin{align*}
& J_{1} \frac{d \omega_{\xi}}{d t}+\left(J_{3}-J_{2}\right) \omega_{\eta} \omega_{\zeta}=M_{\xi}^{(e)}  \tag{5}\\
& J_{2} \frac{d \omega_{\eta}}{d t}+\left(J_{1}-J_{2}\right) \omega_{\zeta} \omega_{\zeta}=M_{\eta}^{(e)}  \tag{6}\\
& J_{3} \frac{d \omega_{\zeta}}{d t}+\left(J_{2}-J_{1}\right) \omega_{\tau} \omega_{\eta}=M_{\zeta}^{(e)} . \tag{7}
\end{align*}
$$

where $\omega_{\xi}, \omega_{\eta} \omega_{\zeta}$ 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 $M_{\tilde{\xi}}^{(e)}, M_{\eta}^{(e)}$, and $M_{\zeta}^{(e)}$ are the projections of the moments of forces on the $\xi, \eta$ and $\zeta$-axis.

Equations (4)-(6) are closed by Euler's kinematic relations, connecting the components of the angular velocity with the Euler angles $\varphi, \psi, \theta$ :

$$
\begin{gather*}
\omega_{\tilde{\xi}}=\dot{\psi} \sin \theta \sin \phi+\dot{\theta} \cos \phi,  \tag{8}\\
\omega_{\eta}=\dot{\psi} \sin \theta \cos \phi-\dot{\theta} \sin \phi,  \tag{9}\\
\omega_{\zeta}=\dot{\psi} \cos \phi+\dot{\phi} \tag{10}
\end{gather*}
$$

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:

$$
\begin{equation*}
M \frac{d v_{f}}{d t}=\sum_{k=1}^{\mathrm{N}-1} \nabla G\left(r_{f k}\right)+\sum_{k=1}^{\mathrm{S}} \nabla \Phi\left(r_{f k}\right), \boldsymbol{v}_{f}=\frac{d \boldsymbol{r}_{f}}{d t} \tag{11}
\end{equation*}
$$

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:

$$
\begin{equation*}
M \frac{d v_{c}}{d t}=\sum_{k=1}^{N} \sum_{i=1}^{S} \nabla \Phi\left(r_{i k}\right)+\sum_{i=1}^{S} \nabla U\left(r_{p i}\right)+\boldsymbol{F}_{p C}, v_{C}=\frac{d r_{C}}{d t} . \tag{12}
\end{equation*}
$$

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

$$
\begin{equation*}
m_{p} \frac{d v_{p}}{d t}=\sum_{i=1}^{\mathrm{N}} \nabla \Phi\left(r_{p i}\right)+\sum_{k=1}^{\mathrm{S}} \nabla U\left(r_{p k}\right)-\boldsymbol{F}_{p C}, \boldsymbol{v}_{p}=\frac{d \boldsymbol{r}_{p}}{d t} . \tag{13}
\end{equation*}
$$

In Equations (11)-(13), $M$ is the fullerene mass; $m_{p}$ is the particle mass; $\nabla$ is gradient operator; $S=60$ is the number of carbon atoms in the $\mathrm{C}_{60}$ molecule; $N=12$ is the number of surrounding fullerenes; $r_{f k}$ is the distance between the center of the considered smoothed fullerene and the center of the $k$ th carbon atom on the inner fullerene; $r_{p k}$ is the distance from the center of the particle to the center of the $k$ th carbon atom on the central fullerene; $r_{p i}$ is the distance from the center of the particle to the center of the $i$ th 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:

$$
\begin{gather*}
t=0: \psi=\psi^{0}, \theta=\theta^{0}, \phi=\phi^{0}, \omega_{\zeta}=\omega_{\zeta}^{0}, \omega_{\eta}=\omega_{\eta}^{0}, \omega_{\zeta}=\omega_{\zeta}^{0}  \tag{14}\\
\boldsymbol{v}_{C}=0, \boldsymbol{r}_{C}=0, \boldsymbol{v}_{f}=0, \boldsymbol{r}_{f}=\boldsymbol{r}_{f}^{0}, \boldsymbol{v}_{p}=\boldsymbol{v}_{p}^{0}, \boldsymbol{r}_{p}=\boldsymbol{r}_{p}^{0} \tag{15}
\end{gather*}
$$

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 $\mathrm{C}_{60}$ fullerene, which is at rest at the initial moment of time. It has a charge $q_{\mathrm{f}}=1 \mathrm{e}$ and an angular velocity $\omega^{0}=0 \mathrm{rad} / \mathrm{s}$ (see Figure 1). The x and $\zeta$-axes coincide at the initial moment of time. Thus, the Euler angles $\psi, \theta(8)-(10)$ will determine the orientation of the $\zeta$-axis in space. At this moment, the incident particle ( $\mathrm{Kr}+, 83.8 \mathrm{a} . \mathrm{m}$.) 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 $2000 \mathrm{~m} / \mathrm{s}$.

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 ( $0.65 \pm 0.02 \mathrm{~nm}$ ) 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 $v_{p}=500 \mathrm{~m} / \mathrm{s}$, a charged particle under the action of Coulomb forces completely loses its speed at a sufficiently large distance ( $x=-2.9 \mathrm{~nm}$ ) and then begins to move in the opposite direction. At $v_{p}=1000 \mathrm{~m} / \mathrm{s}$ for a charged particle, this occurs at $x=-1.45 \mathrm{~nm}$. At $2000 \mathrm{~m} / \mathrm{s}$, 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 center of mass 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 $1000 \mathrm{~m} / \mathrm{s}$. At $v_{p}=2000 \mathrm{~m} / \mathrm{s}$, 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 $670 \mathrm{rad} / \mathrm{ns}$. 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 $10^{2} \mathrm{rad} / \mathrm{ns}$. At $v_{p}=1000 \mathrm{~m} / \mathrm{s}$, 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 $\mathrm{C}_{60}$ molecule at $\omega^{0}=0 \mathrm{rad} / \mathrm{s}$.


Figure 4. Time dependence of the instantaneous angular velocity component $\omega_{\mathrm{x}}\left(v_{p}=1000 \mathrm{~m} / \mathrm{s}\right)$.
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 $\mathrm{C}_{60}$. To overcome the influence causing angular oscillations, fullerene must be given the initial angular rotation velocity $\omega^{0}>1000 \mathrm{rad} / \mathrm{ns}$ (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 $\theta$ in the absence of rotation in other angular directions.


Figure 5. Time dependence of the intrinsic rotation angle $\theta$ for different initial rotation rate of fullerene.

Figure 6a shows that an incident neutral particle with a velocity of $v_{p}=1000 \mathrm{~m} / \mathrm{s}$ increases the maximum rotation speed of the $C_{60}$ fullerene by $1.8 \%$ and $3.6 \%$ for $\omega^{0}=1500$ and $2000 \mathrm{rad} / \mathrm{ns}$, respectively. The charged particle had no effect on the angular velocity.


Figure 6. Time dependence of instantaneous angular velocity: (a) $v_{p}=1000 \mathrm{~m} / \mathrm{s},(\mathbf{b}) v_{p}=2000 \mathrm{~m} / \mathrm{s}$.
At $v_{p}=2000 \mathrm{~m} / \mathrm{s}$, 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 $2000 \mathrm{rad} / \mathrm{ns}$, 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 ( $22.6-23.6 \mathrm{pm}$ ) than in the absence of a charge ( $31.7-35.3 \mathrm{pm}$ ). However, the trajectories of the neutral and ionized particles differ little from each other at $v_{p}=2000 \mathrm{~m} / \mathrm{s}$ (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 $\mathrm{C}_{60}$ 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 ( $\mathrm{C}_{70}, \mathrm{C}_{78}$, etc.) due to their greater mass compared to the $\mathrm{C}_{60}$ fullerene.


Figure 7. Trajectory of the center of mass of the internal $\mathrm{C}_{60}$ molecule at $v_{p}=2000 \mathrm{~m} / \mathrm{s}$.

## 5. Conclusions

In this article, we have presented the hybrid discrete-continuous mathematical model of the interaction between a krypton ion and the $\mathrm{C}_{60}$ 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 $1000 \mathrm{~m} / \mathrm{s}$. 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 $\mathrm{C}_{60}$ 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 $\mathrm{C}_{60}$ 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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