The Dynamic State of a Pseudo-Crystalline Structure of B_{42} Molecules

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Received: 8 May 2020; Accepted: 12 June 2020; Published: 15 June 2020

Abstract: In this paper, we have developed a mathematical model of the dynamics of molecular structures arising from an approach using B_{42} molecules. The model is based on equations that determine the motion of the centers of mass of the molecules in question, and equations for the projections of the moments of quantities of motion of these particles on the axes associated with them. The thermal motions of boron atoms within each individual molecule are calculated using a bond-ordered potential. The intermolecular interactions of atoms have a potential that appears to coincide with that of free atoms. However, the interaction parameters differ. The obtained columns of molecular disks for B_{42} are stable structures. We determine the characteristic vibration amplitudes and rotation frequency of the molecules in question.

Keywords: molecular dynamics; crystals; nanomaterials

1. Introduction

Boron has made a significant impact in our lives through its often unrecognized use in fertilizers, fungicides, soaps, detergents, and heat-resistant glassware [1]. Different applications have stimulated the development of boron science, namely, energy, organic synthesis, petroleum technology, nuclear physics, catalysts, chemistry, materials, and medicine [1,2].

Pham et al. [3] performed quantum-chemical calculations of boron structures by studying the geometry and stability of clusters B_{30}, B_{36}, B_{40}, B_{42}. In this paper, we investigate the structure that can be formed from B_{42} (C_{7}v) and the dynamics of motion of each individual flat disk of B_{42}. Disk B_{42} is a molecule with a thickness of 1 atom. It should be noted that 2D materials or graphene analogs stand out among other materials for their unique properties, namely their excellent physical, chemical, optical, and biological qualities due to their uniform shape, high surface to volume ratio, and surface charge [4]. These properties are necessary for use in various fields, including medicine [5-7], electronics [8,9], mechanics and materials [10], thermoelectricity [11], and others.

Since 2D materials are of great interest, a large amount of work has also been devoted to their synthesis [11,12]. In reference [13], a new two-dimensional all-carbon graphidine was obtained. The following are the properties of some 2D materials. Graphene doped with boron nitride was investigated [14] using density functional theory (DFT). The results show that the formation energy of these systems can increase or decrease with doping. Using DFT analysis, Yin et al. [15] showed that zigzag boron nitrides doped with Fe exhibit semiconducting properties with a direct forbidden band, while the primary nanoribbon from boron nitride is an insulator with an indirect wide energy gap. The same authors, using the molecular dynamics method, report that such iron-doped BN tapes can stably exist in real conditions. In reference [16], the thermal properties of hybrid nanosheets from
boron graphene nitride with various states were studied by the molecular dynamics method. Reference [17] showed the possibility of combining a large volume of boron nitride plates with a small amount of polymer to manufacture plastic. Heat-conducting composite materials for thermoregulation of flexible electronic devices is a difficult task. Reference [18] managed to obtain a sample of polycrystalline cubic boron nitride. In reference [19], the authors study THz detectors based on 2D materials. The analysis performed in reference [20] shows the importance of understanding the influence of a tunable electronic structure on the mechanical response of materials made of carbon and boron nitride.

It is also important to consider other features related to boron. Chauhan et al. [21] discuss boron-based polymers, their capabilities, and applications. Issues regarding the impact of boron on the environment and human health are considered in reference [22]. Yuan et al. [23] obtained coralloid amorphous boron that crystallized upon electron-beam irradiation of the Cu-B-Mg alloy. The resulting boron nanospheres had a size of 5 to 20 nm and exist in an α-B structure. Gas adsorption on nanotubes and fullerenes is considered in reference [24]. Reference [25] reported that boron isotopes give boron arsenide single crystals an unusual and ultrahigh thermal conductivity. Reference [26] performed extensive optimization calculations for B$_{80}$ isomers to find out which principles underlie the formation of large hollow frameworks from boron. Reference [27] reports on the method of growing single crystals of boron arsenide on a centimeter scale. The resulting crystals have unique physical properties. Their modeling showed that borofen can remain more resistant to external mechanical loads than graphene and BN sheets. The authors of [28] state that a polymer-crystalline electrolyte containing anion-trapping boron fragments improves the ionic conductivity of sodium-ion batteries at room temperature. The results show that the adhesion energy for all five of these new allotropes is positive since all of these systems are stable; therefore, these structures can be synthesized in experiments. The possibility of using boron and its compounds for use in hydrogen production and storage systems, in lithium-ion batteries, supercapacitors, and thermal elements is discussed in reference [29].

2. Materials and Methods

In this paper, we consider the relative displacements of B$_{42}$ molecular disks located in a structure that we call a column. To describe these displacements and thermal vibrations, we use a bond-oriented intramolecular potential and a centrally symmetric potential for intermolecular interactions. Thus, we make the completely natural assumption that there are chemical bonds between the boron atoms inside the B$_{42}$ molecule, and there are none between the molecules. The motion of disks as molecular formations obeys the equations of rotational motion and the equations of motion of their centers of mass.

The mesh structures of boron molecules are based on the triangles in Figure 1, as well as pentagons, hexagons, and heptagons. Triangles determine the local structure, and figures with a large number of angles determine the global structure since they are at the periphery of the surface structures under consideration. For example, a B$_{80}$ molecule has a pentagon inside, with a side equal to one B-B bond. It has a pentagon on the periphery, too, but with a side equal to three covalent bonds. The same can be said with respect to B$_{80}$ and B$_{42}$ except that the basis of their designs is the hexagon and heptagon, respectively.
Figure 1. B30 C5v, B36 C6v, and B42 C7v [1].

Assuming that the molecules are deformed during the movement, we write the equations of the theorem on the angular momentum of the molecules for relative motion near their centers of mass:

$$\frac{dK_\xi}{dt} + qK_\eta - rK_\zeta = L_\xi + L^{(n)}_\xi,$$  \hspace{1cm} (1)

$$\frac{dK_\eta}{dt} + rK_\zeta - pK_\xi = L_\eta + L^{(n)}_\eta,$$  \hspace{1cm} (2)

$$\frac{dK_\zeta}{dt} + pK_\eta - qK_\zeta = L_\zeta + L^{(n)}_\zeta.$$  \hspace{1cm} (3)

Here, $L_\xi, L_\eta, L_\zeta$ denote projections of the moment vector of the forces of cross interactions, $L^{(n)}_\xi, L^{(n)}_\eta, L^{(n)}_\zeta$ denote projections of the vector of magnetic forces acting on molecule, $K_\xi, K_\eta, K_\zeta$ denote projections of the angular momentum vector, and $p, q, r$ denote projections of the angular velocity vector. In this case, the projections of the angular momentum vector through the projections of the instantaneous angular velocity vector and the components of the inertia tensor are expressed as follows:

$$K_\xi = A'p - Fq - Er,$$  \hspace{1cm} (4)

$$K_\eta = -Fp + B'q - Dr,$$  \hspace{1cm} (5)

$$K_\zeta = -Ep - Dq + Cr.$$  \hspace{1cm} (6)

Axial and centrifugal moments included in the last relations are expressed by the following formulas:

$$A' = m \sum_{i=1}^{S_i} \left( \eta_i^2 + \xi_i^2 \right),$$

$$B' = m \sum_{i=1}^{S_i} \left( \xi_i^2 + \zeta_i^2 \right),$$

$$C' = m \sum_{i=1}^{S_i} \left( \zeta_i^2 + \eta_i^2 \right).$$

Here, $m$ denotes the mass of any atom in the molecule, $S_i$ denotes the number of these atoms in the described molecule. Equations (1)–(3) can easily be solved with respect to time derivatives of the projections of angular velocities on the moving axes. After that, they are integrated together with
the Euler kinematic relations, which are also resolved with respect to the derivatives of the Euler angles.

The dynamic equations of rotational motion are initially presented in projections on the axis of the moving reference system associated with a single molecule. At the same time, it is convenient to represent the resulting motion in an absolute, motionless coordinate system. In this regard, we construct the absolute basis using the force characteristics: the projections of interatomic interaction forces and their moments at the first stage of calculations. Then, using the rotation matrix, which has components in the form of combinations of trigonometric functions of Euler angles, a transition is made to the projections of the moments of forces in a moving basis. These projections are then incorporated into the dynamic Euler equations. The latter equations are ordinary first-order differential equations with respect to the angular velocities of rotating molecules. The system of these equations will be closed if we include the kinematic Euler relations connecting the derivatives of Euler angles with the projections of the angular velocities and trigonometric functions of the rotation angles. Supplementing all these equations with initial data, we obtain the Cauchy problem for determining Euler angles as functions of time. The dynamic Euler equations are initially presented in projections on the axis of the moving reference system associated with a single B42 molecule. At the same time, it is convenient to represent the resulting motion in an absolute, motionless coordinate system. In this regard, we construct the absolute basis using the force characteristics: the projections of interatomic interaction forces and their moments at the first stage of calculations. Then, using the rotation matrix, which has components in the form of combinations of trigonometric functions of Euler angles, a transition is made to the projections of the moments of forces in a moving basis. These projections are then included in the dynamic Euler equations.

The magnitude of the force acting on a single atom of molecules B42 can be determined as follows:

\[ X_i = -\sum_{i=1, j \neq k}^S \frac{\partial}{\partial x}(U_{bo}(\rho_{ki})) - \sum_{j=1}^S \frac{\partial}{\partial x}(U_{vw}(\rho_{ij})), \]

\[ Y_i = -\sum_{i=1, j \neq k}^S \frac{\partial}{\partial y}(U_{bo}(\rho_{ki})) - \sum_{j=1}^S \frac{\partial}{\partial y}(U_{vw}(\rho_{ij})), \]

\[ Z_i = -\sum_{i=1, j \neq k}^S \frac{\partial}{\partial z}(U_{bo}(\rho_{ki})) - \sum_{j=1}^S \frac{\partial}{\partial z}(U_{vw}(\rho_{ij})), k = 1...S. \]

Here, \( X_i, Y_i, Z_i \) denote projections of the resultant of all interatomic forces directed at the \( k \)th atom of the molecule in question; \( \rho_{ki} \) denotes the distance between atoms inside an individual molecule; \( r_{ij} \) denotes the distance between the boron atoms of various disks; \( S \) denotes the number of atoms in the described molecule, \( S_2 \) denotes the number of atoms located close to the calculated molecule, \( U_{bo} \) denotes bond ordered force field (intramolecular potential), and \( U_{vw} \) denotes the effective potential of interactions between atoms of various B42 disks.

The first group of terms on the right-hand sides of Equations (10)–(12) is responsible for the interaction inside the molecule, and the second group is responsible for cross interactions. The equations of motion of any atom written in the absolute reference frame will have the classical form:

\[ m_x \frac{d^2x_k}{dt^2} = X_k, m_y \frac{d^2y_k}{dt^2} = Y_k, m_z \frac{d^2z_k}{dt^2} = Z_k, \]

\( k = 1,...,S. \)

This theorem can be formulated as follows: The center of mass of the disk B42 moves as a material point having a mass equal to \( 42m_B \) under the action of a force equal to the sum of all cross “atom-atomic” interactions in the system under consideration.

\[ 42m_B \frac{dv}{dt} = -\sum_{j=1}^S \frac{\partial}{\partial r_j}(U_{vw}(r_j)) \frac{dr}{dt} = \mathbf{v}. \]

Here \( m_B \) is the mass of the boron atom; \( \mathbf{v} \) is the velocity of the B42 center of mass; \( U_{vw}(r_j) \) is the potential of cross-actions; and \( \text{grad} \) is the gradient operator.
The right-hand side of the equation of the theorem under consideration does not include forces determined by the gradient of the bond-ordered force field. The latter is due to the fact that internal forces do not change the motion of the center of mass. The diatropic ring current present in the particle [1] causes plate B42 to be an elementary magnet. This allows the system of molecules to fit into columns. Similar processes occur in the blood of a person if red blood cells receive an excess charge for some reason. Conventional magnetic reactions resulting from the movement of electrons through the crystal structure of B42 should not be a reason for refusing to use the classical description of the dynamics of the aggregate of such particles. Magnetic forces of a classical nature enter the right-hand sides of Equations (1)–(3). Differential Equations (1)–(3), (13), and (14) are integrated under the following initial conditions:

\[
\begin{align*}
t &= 0, \quad p = q = r = 0, \\
x_i &= x_i^0, \quad y_i = y_i^0, \quad z_i = z_i^0, \\
\frac{dx_i}{dt} &= u_i^0, \quad \frac{dy_i}{dt} = v_i^0, \quad \frac{dz_i}{dt} = w_i^0 \quad (k = 1, \ldots, S), \\
v &= 0, \quad r = r^0.
\end{align*}
\]

Here, \(x_i^0, y_i^0, z_i^0\) denote the initial coordinates of boron atoms in a single molecule, \(u_i^0, v_i^0, w_i^0\) denote the initial velocity of the thermal motion of atoms. The Cauchy problem (1)–(18) was solved numerically using the fourth-order Runge–Kutta scheme of accuracy and a constant time step \(\Delta t = 10^{-6} \text{ ns}\).

2.1. Algorithm Testing

We mention only three of the tests performed:
1. Inertia rotation of the free disk B42 in three different planes of the coordinate space. If there are no torques, then the initial speed remains constant throughout the movement.
2. Let the velocity vector of the test molecule representing the external action be in the plane of the disk B42 and not directed to its center of mass, which has a fixed position. Then, at the particle approaching site, the disk rotates at a certain angle, and, approaching according to the defined distance, the particle returns to its original position.
3. Two B42 plates located in the same plane but separated by a sufficient distance begin to move towards each other. Subsequently, the movement remains flat. The total energy of the system remains constant throughout the movement. The kinetic energy at the beginning of the test is equal to the kinetic energy of two molecules when they are removed from each other.

All test examples showed an error no greater than 0.01%.

3. Results

Figures 2–9 show the dynamic state calculation data for columns containing two, three, and five B42 molecular disks.

![Figure 2. Rotation angles of two B42 discs.](image)
Figure 3. The angular speeds of the two Bé discs.

Figure 4. The trajectories of individual atoms belonging to different disks.

In Figures 4, 7, and 9, the dimension of the axes is presented in nanometers.

Figure 5. Changes in the angles of rotation of these discs.

Figure 6. Angular frequency of these disks.
Figure 7. Trajectories of nodes located at the edges of three disks.

Figure 8. Angular speeds of 5 discs.

Figure 9. Trajectories of 5 discs.
Figures 2–4 show the results of calculations of the dynamic state of two disks initially located in each other’s potential wells. The calculations were performed without taking into account the influence of magnetic forces caused by the action of diatropic ring currents. Even in this case, the discs are held together, and their movements are symmetrical angular oscillations of large amplitude. As can be seen from Figure 2, the amplitude of these oscillations is about 170°. From Figure 3 it follows that the average oscillation frequency of the two disks is of the order $10^{10}$ s$^{-1}$. With these oscillations, the trajectory of the node of the plate under consideration fills $\frac{3}{4}$ of the circle (Figure 4). Figures 5–7 show the results related to the “coin” column of three disks. As shown in Figure 5, the central disk in its angular oscillations makes almost a full revolution, and the peripheral disks make only half a revolution. This is also indicated by the trajectories shown in Figure 7. Figures 8 and 9 show the dynamic state of a column of five disks. As calculations show, with an increase in the number of disks, the symmetry of motion decreases. Now, the extreme disks make angular oscillations of the greatest amplitude (Figure 9). In this case, the average frequency of angular oscillations remained approximately the same. Along with torsional vibrations, the $\text{B}_{42}$ molecules located in the “coin” column experience small vibrations in the heel and pitch angles (Figure 7). With a further increase in the number of disks in the column, the oscillation amplitude of the extreme disks is $\frac{3}{4}$ of the circle, and the internal disks have the amplitudes $\frac{1}{4}$ and $\frac{1}{2}$. Therefore, the situation shown in Figure 9 is typical. Calculations show that linear stacking of the disks exhibits dynamic stability even if some of the internal disks participate in regular rotations. The latter is achieved by modifying the $\text{B}_{42}$ molecule by introducing an ionizing group of atoms into it, as well as using an external electromagnetic field.

4. Discussion

Calculations show that planar molecules can be combined into “coin” columns. This is facilitated by both van der Waals forces and magnetic forces due to the presence of diatropic ring currents in $\text{B}_{42}$ molecules. However, the resulting linear molecular structures are not static but are characterized by angular vibrations of large amplitude disks. An effective mathematical description of these oscillations is proposed. The angular velocities of the disks in the pseudo-crystalline structures under consideration are determined. Molecular crystals, such as plastic fullerite, have the ability to accumulate energy on internal, rotating degrees of freedom. $\text{B}_{42}$. Molecular crystals that must be obtained from such columns must have outstanding hardness characteristics, since each molecule of such crystals is an elementary gyroscope and prevents access to it. In this study, an application of mechanical methods to describe the rotating dynamics of molecules in molecular crystals is performed. The obtained calculated data can be a guideline when conducting measurements. It is also natural that the best verification of the correctness of the constructed mathematical model is a comparison with experimental data. In experiments, one can record the period of angular vibrations of $\text{B}_{42}$ disks using nuclear magnetic resonance. Similar experiments were performed by Johnson et al. [30], for the case of rotation of fullerenes in the plastic phase of fullerite. In addition, in experiments, it is possible to determine the average distance between the $\text{B}_{42}$ molecules in the columns and the binding energy between the parts of the column, which determines the strength of the considered molecular structures.

Author Contributions: Data curation, Formal analysis, Funding acquisition, Project administration, Visualization, A.B.; Investigation, Methodology, Resources, Software, Validation, M.B.; Supervision, Writing—original draft, Writing—review & editing, D.M. All authors have read and agreed to the published version of the manuscript.

Funding: This work was funded by the Russian Science Foundation under grant No 19-71-10049 and Ministry of Science and Higher Education of Russia (agreement No. 075-02-2020-1479/1).

Acknowledgments: This work was supported by the Russian Science Foundation under grant No 19-71-10049 and Ministry of Science and Higher Education of Russia (agreement No. 075-02-2020-1479/1).

Conflicts of Interest: The authors declare no conflict of interest.
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