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Contents

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Foundations of Thermoelectronics

Stanislav Ordin

A B S T R A C T

The construction of the foundations of thermoelectronics became possible only after the correction of thermodynamic errors in the traditional theory of semiconductor electronics. It was these errors that determined the saturation of the operating parameters of semiconductor electronic devices, in particular, the saturation of the maximum clock frequency of processors. But in semiconductors, although these thermodynamic errors manifested themselves not only in the instrumental, but also in the technological aspect, they did not prohibit semiconductor electronics themselves. It's just that in the theory of semiconductor devices there were a number of qualitative errors that practitioners compensated for with "empirical corrections. So an electronics engineer often made devices not according to a strict theory (which simply did not exist until now), but on a hunch and according to empirical local laws. What was aggravated by the fact that ALL physics was "stuck" on the use of flat electron orbitals, which Pauling introduced for "two-dimensional" graphite and for which he received the Nobel Prize. But, Pauling himself, as an honest scientist, having discovered his mistake, tried to correct it by introducing "curved" orbitals for graphite itself. Now, after the restoration of the Planck-Einstein Quantization, it is shown how to get the correct orbitals instead of the mystical Schrödinger wave functions [1, 2, 3].

1. Stanislav Ordin, «Gaps and Errors of the Schrödinger Equation»», Journal of Materials and Polymer Science (J mate poly sci), 2022; 2(3): p. 1-6.

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3. Stanislav Ordin, "Foundations of Quantization Principles". Jenny Stanford Publishing Pte Ltd, 2023, 235 pp.

Keywords: *Thermoelectronics, semiconductor electronics, Stanislav Ordin*

Introduction

The dimensional thermoelectric effect in silicon carbide crystals, which I initially discovered back in the 1980s, showed insufficient completeness of thermoelectric phenomenology to describe thermo-EMF and output resistance in microstructures with potential barriers (Fig. 1).

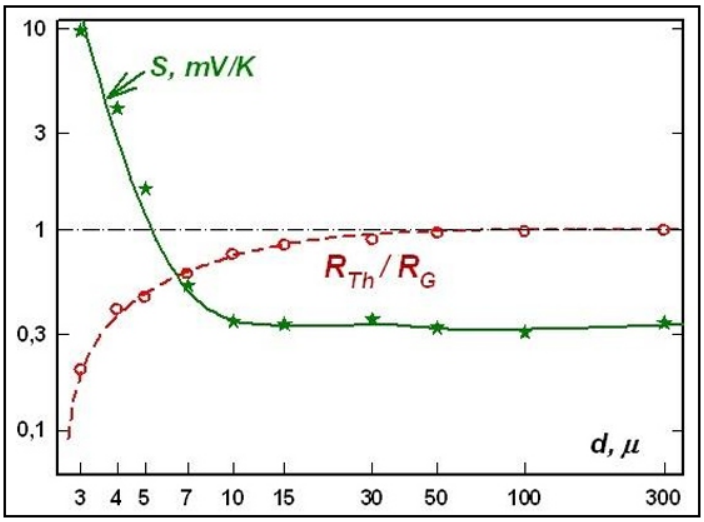

Fig 1: Dependences of thermo-EMF (originally it was believed that this is the diffuse Seebeck coefficient) and the ratio of the output thermoelectric resistance to the galvanic resistance of a SiC semiconductor crystal depending on its size (thickness along the heat flux)

But a rigorous theoretical extension of the purely diffuse (as analysis showed) theory of thermoelectricity was made by me later. And then, neither the laboratory of thermoelectricity of the Ioffe Institute, nor the international thermoelectric community dared to deviate from traditional thermoelectric concepts and with the need to correctly take into account the concentration force. Take it into account as it is done in the pn junction theory. And the management of the Global Thermoelectric company, which arranged a radio conference with me at the beginning of this century, summarized both our discussion and the general position of the thermoelectric community by saying: “We are now the world's largest manufacturer of thermoelectric generators using wellestablished traditional technology. And where will we be if we switch to the Intel technology you propose for thermoelectricity”.

But even then, albeit at a qualitative level, I already felt that there is a “reverse side of the coin”, that phenomenology and as a result, calculations of the characteristics of the p-n junction are also not complete without taking into account the temperature force traditionally used in thermoelectricity. I understood, showed at a qualitative level to the management of Intel that it was precisely because of taking into account the temperature force that they reached the saturation of the processor clock frequency with an increasing miniaturization of individual elements (an increase in the number of elements in a chip). But Intel, for its part, was afraid to move away from the traditional technology for manufacturing processors, and tried not to solve the problem correctly, but to get around it due to multi-core. But this method of increasing the number of elements, even then it was obvious, would not allow going beyond the logarithmic dependence of the speed of processors on the number of elements in them. Now my early qualitative calculations have received rigorous confirmation in the expansion of electronics to thermoelectronics.

Historical errors of semiconductor electronics and their correction

The historical consideration of electronics without taking into account heat flows has imposed a number of restrictions on the design of devices and devices based on it. In addition, they led to a number of "theoretical" bans on the existence and the possibility of registration, which was revealed in the study of the previously described Local thermo-EMF. At the same time, before turning specifically to polymers, it is necessary to make a significant clarification. Lack of understanding of the physics of Local thermodynamic effects not only imposed a ban on the Local Effects themselves, but also led to a false attribution (even. WIKIPEDIA) of the device to a photo-thermoelectric converter, while it contains asimple photo-conversion of the thermal radiation flux. This happens in Science, unfortunately, not infrequently. The ideas of its Creators are not fully understood, but picked up by the developers, they are actively moving forward, but with distortions and errors. So, now that the fundamental sections of Physics have reached the modern level, it became clear that an entire industry has been formed-electronics, the instrumental and technological problems of which are related to the fact that the theory of p-n junction is built in violation of the laws of non-equilibrium thermodynamics and that this is largely determined by distortion Ideas that the Founders of electronics came up with purely intuitively.

So, it is in the p-n junction, first discovered in silicon carbide and described in the 30s of the last century by Oleg Losev, who himself immediately intuitively realized that this was a current device. And he was able to use it almost immediately: he created on it an LED, a photodiode, and a resistance transformer, which the Nobel laureates called in short (in English) a transistor. But the physics of the p-n junction and the description of the operation of the listed devices based on the p-n junction were built by analogy with a radio tube, which, in principle, is a field device. Thus, when solving various problems for semiconductor devices in the p-n junction, the cause-current and the effect-voltage were rearranged. And the prominent physicist Abram Fedorovich Ioffe did not fully understand Losev then, who was half a century ahead of modern electronics. But Academician Ioffe, not like the current "luminaries of science", succeeded in conferring on him a candidate of physics and mathematics. sciences without defending a dissertation. And only after almost 100 years, the return to Losev's current circuit made it possible to significantly improve the characteristics of semiconductor devices.

Tauc is another, Czech Corypheus, ahead of his time. He was the first, immediately after the liberation of Prague by the Soviet troops, to establish the production of point transistors in Prague (formerly of the Bell company). And he immediately discovered thermoelectric effects in the p-n junction and honestly described them. But thermoelectricity itself was then (and still is) stuck at the macroscopic level and relegated Tauc's results to the category of anomalies. The thermodynamic discovery by Ilya Prigogine of the production of local entropy helped to restore the correct description of the physics of the p-n junction, which made it possible to understand that in the p-n junction, described for the reasons noted above, within the framework of a truncated concentration-electric phenomenology, it is necessary to use an extended phenomenology supplemented by a heat flow [123]. The standard band structure of the transition itself (Fig. 2a) is modified when the temperature force is taken into account.

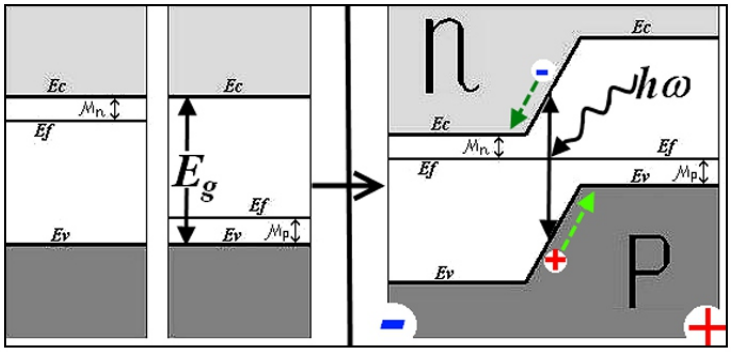

Fig 2a: The traditional scheme for the transformation of energy bands of semiconductors with different types of conductivity upon their contact and the opening of the p-n junction formed in this case when the i-region is irradiated with light

At the same time, the energy diagram of the equilibrium p-n junction is somewhat modified, which, without taking into account the temperature force, gave, as shown in Fig. 1, the potential barrier value approximately equal to the band gap of the semiconductor. Taking into account the temperature force, in the absence of a heat flux, the value of the potential barrier turns out to be equal to half the band gap (Fig. 2b). And when it turns on the heat flow, the value of the potential barrier will increase until a tunnel breakdown occurs (Fig. 2).

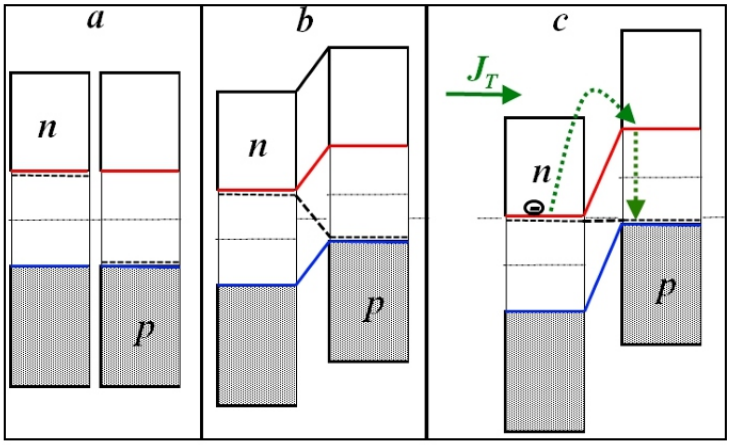

Fig 2b: Energy diagrams of two semiconductors of different types of conductivity: a-before bringing them into contact, b-equilibrium state after their contact at equal temperatures, c-equilibrium state with heat flow through the p-n junction

As shown in Fig. 2b, between semiconductors brought into contact in an equilibrium state due to the balance of electric and concentration forces, the difference in electric potentials at the contact (red line is the bottom of the conduction band, blue line is the top of the valence band) is equal in magnitude and opposite in sign to the difference at the boundary of the concentration potential (dashed black line). Thus, given in Fig. 1b, in accordance with the complete system of equations for thermodynamic forces and flows, it already allows eliminating the theoretical equal to 2 in the description of the transition without a temperature gradient, which was associated with an empirical coefficient due to the imperfection of materials. The potential difference across the transition plates is equal in this case to half the band gap. And the equality of concentration potentials corresponds to the Local Thermo-EMF and occurs, of course, only with a heat flow through the transition (Fig. 2c). In this case, the currentvoltage characteristic (CVC) of the p-n junction, of course, depends on the temperature difference on its plates (Fig. 3). And on the I-V characteristic of the upper left quadrant, a region of positive currents arises at negative voltages at the pn junction, which, in full accordance with the concepts of generators (the simplest-an electric battery), is the region of electric energy generation due to the flow of heat flowing through the junction.

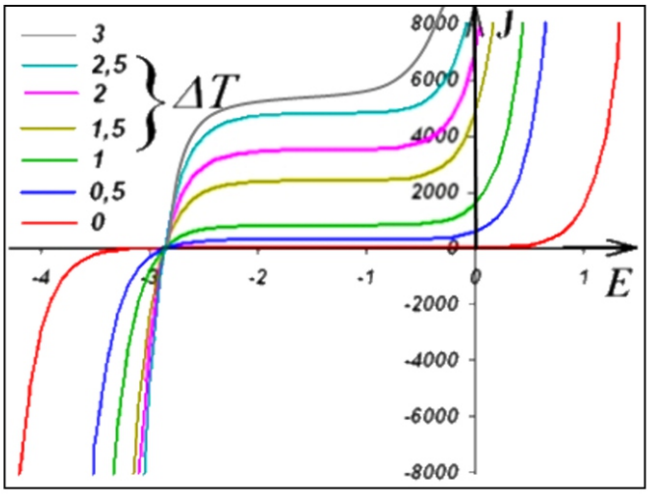

Fig 3: Generator characteristic of a p-n junction, showing its tunneling self-breakdown

The oscillator characteristic of the transition is constructed without taking full account of the specifics of the equilibrium state, taking into account the local production of Prigogine's entropy. In this case, zero current through the junction corresponds to a zero-temperature drop. But in fact, the p-n junction is Maxwell's demon-a "gear" wheel separating hot and cold current carriers, in principle, allowed at the

micro level by the production of Prigogine's Local Entropy. And the mechanism of its operation is obvious from Fig. 2: when semiconductors come into contact, its asymmetry (polarity) occurs. At the same time, to start the electron transfer process, an energy equal to half the band gap is sufficient, while after their transfer and annihilation with holes, their reverse transfer requires an energy equal to the full band gap. So, a local temperature drop occurs on the plates of the p-n junction, which determines the local thermodynamic equilibrium. In this case, the experiment shows that the CVC has a shape fundamentally similar to that shown in Fig. 3. The use of extended concentration-electrical-thermal phenomenology made it possible to correctly take into account Losev's current p-n junction, and to transfer the "anomalous" thermoelectric power discovered by Tauc in the p-n junction to the category of normal-local, and to describe new experimental results of studies of contact thermoelectric power. In addition, the extended phenomenology made it possible to understand that macroscopic thermoelectricity is artificially limited only by diffuse thermoelectric materials and showed that for diffuse thermoelectrics, the efficiency of thermoelectric conversion achieved in practice is already close to the theoretical limit.

In addition, extended phenomenology has shown that the efficiency of thermoelectric conversion based on local thermoelectric power has no diffuse limit and can be dramatically increased by several times compared to that achieved using the Seebeck effect in traditional diffuse materials (Fig. 4).

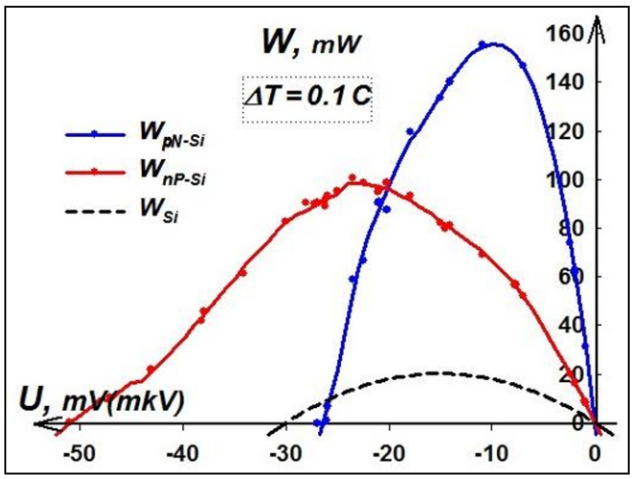

Fig 4: Thermo-generator characteristics of p-n junctions and optimally doped silicon (for silicon, the optimal EMF-μV is three orders of magnitude lower than that of p-n junctions-mV)

This was experimentally confirmed on the developed detectors based on Local Thermo-EMF in silicon junctions, the volt-watt sensitivity of which was obtained three orders of magnitude higher than that of detectors based on the traditional macroscopic Seebeck effect. At the same time, the extended phenomenology shows that there can be complex, three-phase effects in the p-n junction, which makes it possible to optimize, in particular, the combination of local thermoelectric effects with photoelectric effects in it.

Conclusion

The study of Local Effects raised a number of fundamental questions that ended up in a fork: from-this cannot be, to thiselementary. This also applies to the registration of detected and previously referred to as anomalous Local thermo-EMFs, but not only.

But by and large, it is the ELEMENTARY Solution, in contrast to the Primitive, that allows you to create devices with fundamentally (dramatically) improved characteristics. This was the case before, when new devices were created based on the well-known First Principles, the same was confirmed when creating detectors based on the discovered NANO-effects, the study of which resulted in the previously missed NANO-Physics.

Thus, in order to achieve this cardinal improvement in the characteristics of devices and devices, it was necessary to solve a number of fundamental issues and a number of methodological measurement issues, and a number of issues related to the technology of manufacturing efficient semiconductor nanostructures, and a number of design issues.

Within the framework of this study, answers were obtained to a number of fundamental questions

1. Measurability of Local Effects.
2. The primacy in the effects of the current as the cause of the effect and the secondary nature of the voltage, as a consequence, taking into account external conditions.
3. Electric currents semiconductors. over potential
4. Thermal force in the p-n junction.

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In the Scottish café (Polish: Kawiarnia Szkocka) house, the academic scene, a mathematician Stefan Banach and the Scottish book

Mohsin Ahmad Dar and Rajni Bhargav

ABSTRACT

Mathematicians from the Lwów School of Mathematics collaborated to address research issues, in the paper the academic scene of Scottish Café, particularly in functional analysis, topology and mathematical problems, further how Stefan Banach come across with other mathematicians. This paper also discusses the Scottish Book, a large notebook used by Polish mathematicians at the Lwów School of Mathematics to record issues that they intended to answer. The "Scottish Café," where the journal was stored, inspired its name.

Keywords: *Lwow, Stefan Banach, mathematics, Scottish book*

1. Introduction

In the 1930s and 1940s, mathematicians from the Lwów School of Mathematics collaborated on research problems, particularly in functional analysis and topology, at the Scottish Café in Lwów, Poland (now Lviv, Ukraine).

According to Stanisaw Ulam, the café's tables had marble tops so that they could take notes while conversing directly on the table. Stefan Banach's wife gave the mathematicians a large notebook, which was used for writing the problems and solutions, and which eventually came to be known as the Scottish Book, in order to prevent the results from being lost and because she got frustrated with their writing directly on the table tops. The book, which was a collection of issues that had been resolved, unresolved issues, and even issues that were unquestionably intractable, was available for checkout by any customers of the café [1].

2. The Academic Scene

Unfortunately, because there is so little history to recount, it is very simple to place the Lwów School of Mathematics which was born at the Scottish Café in the context of Polish mathematics as a whole. Poland had been divided among Austria, Germany, and Russia since 1795. As a result, it mainly missed the sciences rapid development in the 19th century. Literature and poetry were crucial for promoting the idea of independence and even for the language's preservation in the 19th century, according to Zelazko, who writes that “the primary effort of the nation was given to the humanities.” [2] He claims that because the mathematical work was written in Polish, it was lost to the rest of the world.

When World War I came to a conclusion, the partition was resolved, and a revived Poland sprang into vibrant intellectual life. The cities of Warsaw and Lwów were the main forces behind this mathematical renaissance. Under Zygmunt Janiszewski's leadership, the new publication Fundamenta Mathematicae at Warsaw University became the first specialised journal in the subject of mathematics. Sadly, Janiszewski passed away just as issue one was being typeset.

The University and the Polytechnic were the two educational facilities in Lwów that were relevant to mathematics. In 1661, the Jan Kazimierz University, as it was then known, was established. The University had 5,900 students enrolled in its five faculties in 1934–1935, 870 of whom were in the Mathematical Biological Faculty. Roman Catholicism made up 64% of the larger religious organisations, followed by Judaism (21%), and Greek Catholicism (13%). In the beginning, the Polytechnic was founded in 1816. It was known as Lwów Polytechnic School throughout the interwar period and Lwów Polytechnic beginning in 1921 [3].

Both of these institutions the Polytechnic and the University were seen as having equal worth. People appeared to transition between them with ease, adhering to specific professors or ideologies. As a result, it is difficult to distinguish between employees and institutions. People would attend one to study and attend the other to become a professor or instructor. Students would go to either or both lectures. The literature gives off the strong sense that the Lwów students were genuinely passionate about their studies. Mathematical conversations would erupt outside of the lecture halls and into the cafes and streets. There have been mathematical tea parties. Students would frequently go to each other's homes to discuss mathematically related subjects. Memoirs regularly discuss the ferocious atmosphere that surrounded this most enigmatic of themes, not just in Lwów but also in Warsaw and Krakow.

The Lwów School was largely influenced by a spirited mathematical conversation that took place in Kraków's Planty Park in 1916. In their 20s, Stefan Banach and Otto Nikodym were conversing about the Lebesgue integral while sitting on a park bench. They had a strong commitment to it. There was an uproar. Hugo Steinhaus, a lancer in the Polish army and holder of a doctorate in mathematics from Gottingen, went by in sharp military attire. He stood up and introduced himself as he watched the two argue [4]. Later, Nikodym and Banach travelled to Lwów to enrol in Steinhaus' Lwów Polytechnic. Nikodym went on to have an illustrious career as a Professor of Mathematics in Warsaw and then in the United States of America. Stefan Banach became Stefan Banach

3. Stefan Banach

It took some time before Banach's brilliance in mathematics was acknowledged. His early years had not been very favourable. His mother was unknown, while his father Stefan Greczek worked as a railway official (his surname comes from a laundress, Katarzyna Banach, who played no further role in his life). Years later, Greczek revealed to his renowned son that he was unable to wed his mother due to his financial situation. Stefan was a young man who lived in careful poverty. He began instructing when he was still a student. He didn't ever quit.

We will never know if the Lebesgue integral conversation in Planty Park was actually a tutorial by Banach, but one crucial outcome was that he had a friend in Steinhaus who had gone on to become a professor there when he arrived to study at the Lwów Polytechnic. With Steinhaus' assistance, Banach eventually rose through the University's ranks to become an assistant professor, a professor, and then the Faculty Dean. This was despite the fact that he had no formal education; after struggling to pass his high school exit exams, he only finished two semesters of university study.

However, it made little difference because Banach was manifestly unique. He was given a challenging challenge to tackle by Prof. Steinhaus shortly after his arrival at Lwów, which he accomplished in a single day with ease. Their first joint publication was based on the solution, and they continued to work

together after that, co-authoring papers, founding a math journal (Studia Mathematicise), and contributing problems to the Scottish Book. Banach got married to Lucy and continued his career. Life was good.

He truly was an original. The fact that he was tall, blond, and blue-eyed, informal, and perpetually broke (academic salaries were a joke), led him to leave his previous position in the Café Roma and move across the street to the Scottish Café. The Lwów School of Mathematics at The Scottish Café was centred around Banach. He was employable anywhere. He wasn't bothered by noise. His favoured working position was near to the orchestra in concert halls. He continued thinking with his renowned lucidity. He enjoyed drinking cognac and coffee and conversing about mathematics with nearly anyone while relaxing in the Scottish Café, but you had to be prepared for it since he didn't put up with fools. In contrast to the dapper Prof. Steinhaus, Banach was more casual, to the point where his short-sleeved shirts, lack of a tie, and approachable demeanour with students were viewed as everything but professorial.

However, it was his influence and his relentless pursuit of concepts and answers that fuelled the Lwów School of Mathematics. The first few meetings were sporadic, but after that they began to follow a predictable, daily schedule. Mathematicians crowded inside the Scottish Café. Herman Auerbach, Stanislaw Mazur, and Stanislaw Ulam, three of Banach's prize pupils, were seated at the head table with him every time, but many other people joined them; some of them went on to become well-known around the world. There are almost 30 mathematicians affiliated with the Lwów School of Mathematics, and it is outside the scope of this paper to go into more depth about any one of their lives or bodies of work than is necessary. What were they discussing? In line with Ulam [5]:

The set theory subfields the foundation of set theory, set topology, and later under the influence of Banach and Steinhaus functional analysis with applications to classical analysis were the primary drivers of the original research endeavour. In his lectures at universities, Schauder focused on partial differential equations. His techniques and outcomes are still widely used today. The widely used approach to solving analysis problems by applying geometric methods of function spaces was developed by Banach, Mazur, and Schauder. It became standard practise to formulate ideas as problems and then share them in what became the American “brainstorm” developed years later as a formal technique at Los Alamos by Ulam, von Neumann, and others [6] as the mathematical conversations in functional analysis, set theory, topology, and probability grew wider and deeper.

someone drew a straightforward figure or put characters like on the tabletop. This heuristic frequently resulted in the formulation of novel issues or the creation of new mathematical paradoxes. Most frequently, Banach, Ulam, or Mazur arrived at the café with a well stated issue. The journey started. The session's attendees made an effort to consider the problem. Their minds were free to stray throughout Banach's rooms. There were extended periods of thought, focus, and tension. They either thought logically or intuitively. Banach was a computer that processed information instantly, but not everyone could keep up. He did not like to walk around the beaten tracks, but he looked for new ways, looked for distant and surprising associations, often looked into each other's eyes, drank coffee or cognac, burned out a lot of cigarettes: they drank too much, they smoked too much, and time seemed to have stopped.

What a beautiful representation of group thinking - this brooding group of men (at the time, there were no female mathematicians on the faculty), focused, muttering the odd comment, engrossed in the issue. After that, [6]:

Often it happened that one of the scholars -sometimes Banach, sometimes Ulam. sometimes Mazur – experienced a revelation… Like a flash of light, there was the initial idea of a solution. If it was an interesting trail, they would write it on a table top or on napkins. Together, they experienced a feeling of joy and relief, satisfaction and pride. Then they tried to prove the claim using the deductive method. Table tops were densely covered with mathematical signs. When Banach saw that they were beginning to err, he never expressed strong opposition. Rather, he posed new questions, made gentle remarks that often allowed him to find the right path. Apart from illustrating the method, this quotation points to the very real need for The Scottish Book.

4. The Scottish Book

Armed with soft lead pencils, the mathematicians entered the Scottish Café. These were used to target the marble table surfaces, which were simple to write on and, more importantly, easily erasable. According to one commenter, The Scottish Café was set up in the Viennese style. They found it very helpful to utilise little tables with marble tops as slates that they covered in numbers. Initially, this did not cause the owner to express excessive joy, but over time, Zielinski grew accustomed to this "ruination" of his land. After all, serious university and polytechnic professors were seated at the tables rather than juvenile idiots [6]. After one of Banach's tremendous evening spurts of mathematical brilliance had passed by the next morning, according to Urbanek [7].

When Professor Lomnicki first entered the room, he instructed everyone to "always leave the writing on the table as it is and store the table somewhere till the next day" in case it happened again. The tables that had been marked up were then covered with a cloth and placed aside. Cleaning crews were instructed not to wipe such tables when they arrived in the morning, and around 11 o'clock a student would enter and write down the shambles. In a pinch, this method worked, but nobody was pleased with the results.

In 1933 or 1934, we resolved to give our existing formulation of the issues and conclusions of the discussion a more lasting form, according to Ulam [8]. The decision-making procedure is described in the following way by Bakula. Tomasz Zieliski, the proprietor of the Scottish Café, came up with the notion of how to save all these theories, questions, and difficulties so that they would not perish for ever. He could simultaneously defend the priceless marble tops from being destroyed by the pressure of lead and water. This is the account of how one of the greatest books in mathematics history came to be [9]. Rakhiel clarifies the origin myth as follows: Indelible pencils ruined marble tables, and the cafe owner complained about it to Banach's wife [10].

The words "Ksienga Szkockza" (The Scottish Book) were scratched on the top page by someone, perhaps Banach since it was his notebook and he had given the first problem. After that, pages were filled in with a problem on the left and any solutions (if there were any; many problems are still open today) on the right. The date was entered, along with the names of the problem creator and solution. Small rewards were given out for solutions, including a bottle of wine, five beers, and a live goose, which was given to Per Enfilo of Sweden in 1972 when he submitted a negative answer to problem 153. Mazur. Although the awards imply some lightheartedness, adding issues to the novel was not an impulsive decision. Prior to being considered for "formal" inclusion into the "Book," Ulam stated that "the majority of the submitted issues were expected to have had considerable attention given to them." [8] This explains why it has remained relevant and durable [11].

Despite the claim that the book has 193 numbered problems,there were a few more. Some had no numbers, and others were advertised as second or third instalments of earlier issues when they were actually brand-new. There are 198 problems in according to Duda [12]. Thirty mathematicians contributed, with Banach, Mazur, Ulam, and Orlicz dominating the area in the early years and Schreier, Auerbach, and Steinhaus also making significant contributions. The first few years are concluded by Kuratowski, Schauder, Ruziewicz, and Lomnicki. Later authors include well-known foreigners such American John von Neumann and Cyril Offord, the first mathematics professor at the London School of Economics.

Divergent views exist regarding the caretaker of the Book in the Café and the location of its hiding place while not in use. The headwaiter is mentioned as the guardian who "would, upon demand, fetch it out of some secure hiding spot, leave it at the table, and when the guests had left, restore it to its secret location." [8] According to Ulam, This notebook was stored at the Cafe and was brought by the waiter upon request. We filled out the problem, and the waiter dutifully returned it to the location where it was hidden [10]. Hugo Steinhaus asserts that the Scottish Book was kept by a hired employee rather than the cloakroom attendant, a waiter, or the owner [4], although Bogdan Mis maintains that the book was "stored in a cloakroom and provided to mathematicians on request: anyone may post a solution to a problem." [13] The Book was presented to the proprietor, Tomasz Zielinski, after the café had closed, who "handled it extremely carefully. He obviously appreciated its historical significance. [10]. As the years passed, the mathematicians at the Scottish Café kept up their mental gymnastics and added the results of their talks and thought experiments to the book. Many of the righthand pages included answers, whereas the left-hand ones mostly contained questions. In the cited literature, a thorough examination of the book and its multiple authors has been done.

The book thus proven to be beneficial for both the discipline of mathematics and Mr. Zielinski's marble tables. The book still has unquestionable significance as a store and source of unresolved problems, and the findings from this work have influenced a significant portion of current mathematics.

5. Conclusions

This paper focuses on a mathematician Stefan Banach story and his conversations with other great mathematicians in the Scottish Café in the years. The mathematicians initially relates the practical applications of mathematics in subsequent years and mathematicians discussed research problems, particularly in functional analysis and topology from the Lwow School of mathematics. Also, describes the suggestion on "The Scottish Book".

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Modern method for determining the specific activity of natural radionuclides

Shaxzod Turabekov

A B S T R A C T

The purpose of this work is to get acquainted with the basic properties and laws of interaction with the substance of gamma radiation. The practical part of the work includes an acquaintance with the technique and technique of gamma-ray spectroscopy by the example of recording the gamma spectrum of a Cs137 preparation with a spectrometer with a scintillation detector, followed by calibration of the energy scale. After that, on a calibrated spectrometer, it is proposed to determine the attenuation coefficient and estimate the energy of gamma quanta.

Keywords: *Scintillation, radiation, chemical bond energy*

1. Introduction

The term gamma radiation appeared in the analysis of types of radioactive radiation: this is how (γ is the third letter of the Greek alphabet) the radiation of radioactive nuclei, which is not deflected in a magnetic field, was named. Gamma radiation is electromagnetic radiation that accompanies the transition of nuclei from a state with a higher energy to a state with a lower energy. The energy range of photons (γ-quanta) conventionally begins with energies of the order of 103 eV (λ < 10-9 м). Thus, the lower limit of the γ-ray energy range overlaps the X-ray energy range.

Gamma radiation is also called bremsstrahlung of fast charged particles; Electromagnetic radiation arising from the decays of elementary particles, during the annihilation of a particle and antiparticle: Electromagnetic radiation contained in cosmic rays. In these cases, the radiation is also gamma radiation, although there is often a name indicating the cause of its occurrence: bremsstrahlung, annihilation radiation, synchrotron radiation. The upper limit of the energies of gamma quanta emitted by nuclei - products of alpha and beta decays, is about 107 eV (λ ~ 10-13 m). 3) Photon participates only in electromagnetic interaction. The electric charge is equal to zero, as a result of which the effective cross section for the interaction of a photon with charged particles is much smaller than the cross section for the interaction between charged particles. The consequence of this is the greater penetrating power of gamma radiation compared to the penetrating power of the flow of charged particles.

Accordingly, radiation with characteristics 2J and P= (–1)J is called electric 2J - field (EJ) radiation, and radiation with characteristics 2J and P =(-1)J+1 - magnetic 2J - field (MJ) radiation. Radiations with J = 1, 2, 3, 4 are called dipole, quadrupole, octupole, hexadecapole, respectively.

The properties of the EJ and MJ radiations are similar to those of the radiations of macroscopic distributions of charge and currents, for example, a Hertz dipole (E1), a frame with a current (M1), antenna devices of various types.

Let us consider the main laws governing the gamma activity of radioactive nuclides. During radioactive decay, the product nucleus with a certain probability may appear in one of the excited states (Fig. 1). The transition of the nucleus to lower energy levels is accompanied either by the emission of a gamma quantum (radiative transition), or by the transfer of energy to an electron from one of the inner electron

shells (K, L) of the atom, which is emitted from the atom with kinetic energy:

$Ee = E - Ei$

where E is the nuclear transition energy, Ei is the ionization energy of an electron. This process is called internal conversion, and the transition - conversion transition.

The ratio of the probability of a conversion transition to the probability of a radiative transition is called the internal conversion coefficient α. The range of possible values of the internal conversion rate: $0 < \alpha < \infty$.

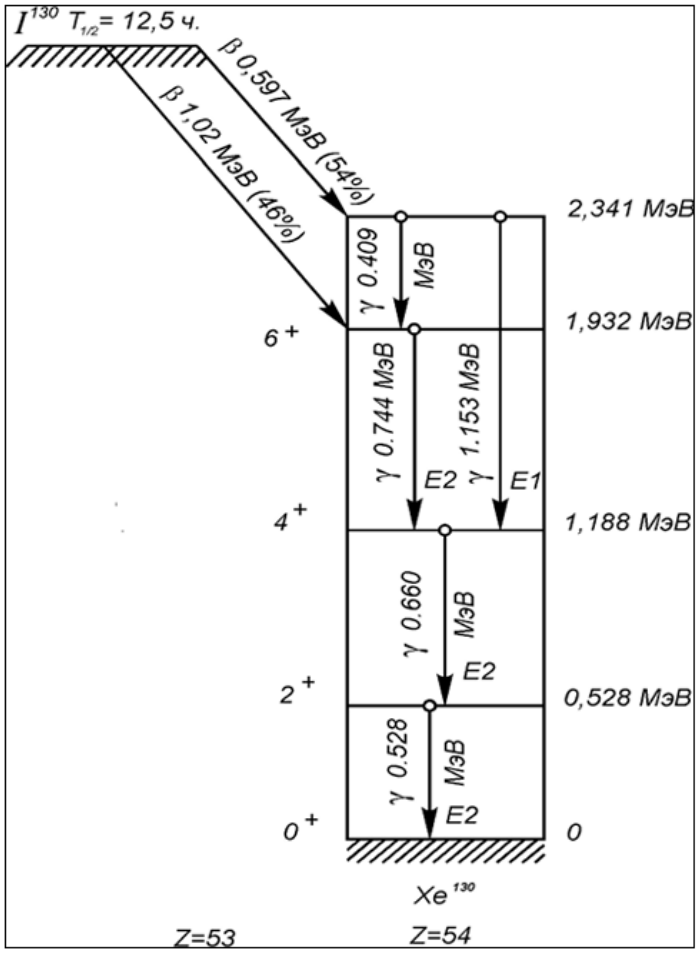

Fig 1: Schematic of the decay of the I^{130} Nucleus

Gamma absorption processes

The absorption of a photon by a free particle, without changing the rest energy of the latter, that is, when the photon energy is converted into the kinetic energy of the particle, is impossible, since the laws of conservation of energy and momentum are not simultaneously fulfilled. The electron has no excited states, its rest energy is unchanged, therefore, free an electron cannot absorb a photon at any energies of the last. Absorption processes gamma quanta occur with the participation of mediator particles. There are two mechanisms for the absorption of gamma quanta: the photoelectric effect and the production of electron-positron pairs.

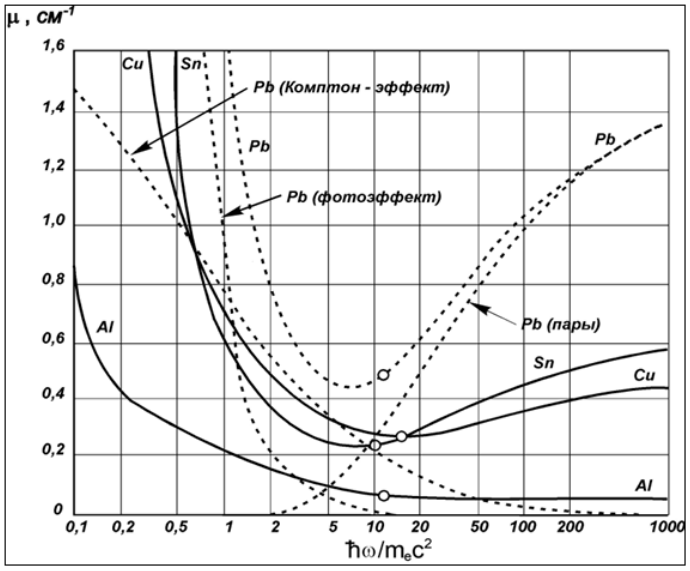

Fig 2: Dependence of the absorption coefficient on the energy of the γ-quantum.

To calculate the amount of energy transferred by gamma radiation to an absorbing medium, it is necessary to take into account that the contribution of each of the interaction processes is different. With FE, almost all the energy of a quantum is transferred by the photoelectron to the atoms of the medium; with Compton scattering, a significant part of the energy is carried away by the scattered quantum to the neighboring regions of the medium or beyond, some of the scattered quanta undergo secondary scattering or absorption; in the processes accompanying REPP.

Scintillation counter

The assembly of the scintillation counter consists in a rational combination of the scintillator and photomultiplier, which would provide the best resolution of the counter, both in amplitudes and in time, at the highest ratio of the amplitudes of electrical pulses from the detected particles to the amplitudes of the background pulses. A scintillator in the form of a cylinder or a disk is installed in front of the PMT cathode. For the fullest possible use of the light arising in the scintillator, the free surface of the latter is surrounded by a diffuse reflector, most often finely dispersed powder of magnesium oxide is used (reflection coefficient 90-97%). A good optical contact is created between the scintillator and the photomultiplier photocathode using a substance with a refractive index intermediate between the glass and the scintillator substance. When registering low-energy particles, measures are taken to reduce the absorption of particles in the scintillator package. Light flashes in scintillators when they are irradiated with quanta arise as a result of the interaction of secondary electrons (appearing due to FE, REPS, and EC) with scintillator atoms. The intensity of the flares will be proportional to the energy of these secondary electrons. Let us consider the picture of the distribution of the energies of secondary electrons.

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An overview of theoretical investigations on interaction of drug molecule with functionalized carbon nanotubes as drug delivery system

Kumara Dhas M

ABSTRACT

CNTs are promising nano-carriers for both drugs as well as biomolecules. This study possesses in-depth knowledge and understanding of carbon nanotubes both for their pharmaco-toxicological properties in drug molecule, it is essential to recommended for routine clinical use in the form of drug delivery carriers in the diagnosis and treatments of many diseases. The surface modified or functionalized Carbon nanotubes (CNTs) can be used for different purposes like improving solubility, carrying various therapeutic, and targeting agents. The functionalization of CNTs can be done via covalent or noncovalent bonding. The Density functional theory calculations are very much helpful to understand the effects on covalently binding of drug molecule with functionalized carbon nanotubes and fullerenes. The present review focus on the structural stability of drug molecule and adsorption behaviour of molecules over various types of CNTs. In addition, progress in carbon nanotube technology may well lead to better insights into biological and physical chemistry processes through theoretical calculations. This will make it possible to find drug molecules more compatible with carbon nanotube to facilitate in medical field.

Keywords: *Carbon nanotubes, drug molecule, density functional theory*

1. Introduction

Nanotechnology is a wide area of research; it deals with a variety of materials produced at a nano-meter scale through different chemical and physical methods. The nanostructures can be used for application in targeted delivery of drugs and encapsulation of both hydrophobic and hydrophilic substances, drug stability is enhanced &provides site-specific delivery [1, 2].

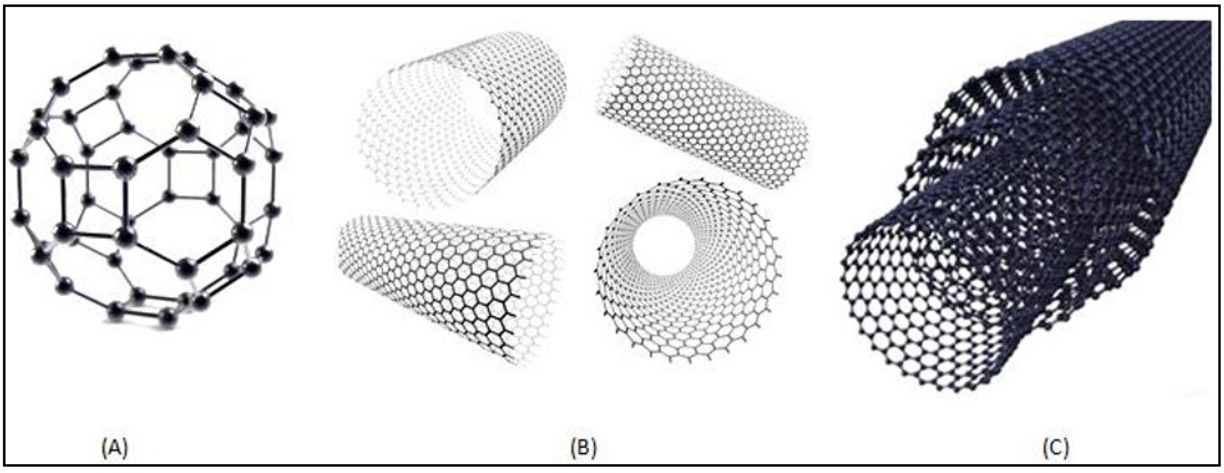

Fig 1: Classification of carbon nanotubes

Carbon nanotubes (CNTs) are tube-like materials, made up of carbon with a diameter on a nano-meter scale. Recently, CNTs have been widely used to deliver therapeutic agents to the targeted tissues and cells due to their physicochemical properties. The application of CNTs in various disciplines like nanotechnology, transistors, nanomedicine, biosensors, bioimaging, actuators, and condensers. CNTs can be classified into various types based the numbers of graphene sheets layered either single layered,

multi layered or double layered as well as also as nanotubes based on chirality i.e. Single walled, multi walled, shown in Figure 1.

The good compatibility of CNTs functionalization helps to reduce systemic toxicity and improves the efficacy of therapeutic agent delivery. Carbon nanotubes are most exploited for various applications, which interacted with biomolecule, drug, and drug delivery to the targeted organs, biosensor diagnostic and analysis [3-5].

In this review, an overview of properties of carbon nanotubes on different clinical applications of CNTs such as disease diagnosis and drug targeting are discussed. The review mainly focusses on the basic structure of CNT, their functionalization, and interaction of drug and biomolecule nanocarrier system by means of density functional theory calculations.

2. Density functional theory Calculations

As a block diagram, the drug delivery mechanism is as shown in Figure 2.

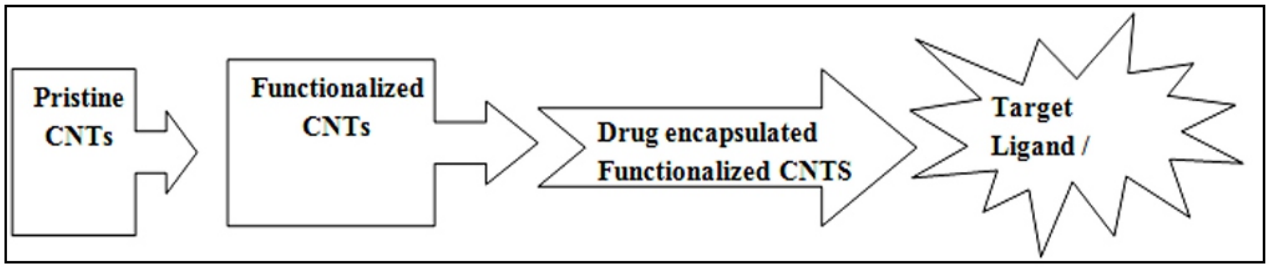

Fig 2: Drug Delivery Mechanism

Nagarajan et al. reported the first-principles studies on interaction of the flutamide (FLU) drug onto graphdiyne nanotube (Gdn-NT), and the favorable interaction sites of FLU on Gdn-NT, the results of the study recommend the use of Gdn-NT as a drug-delivery vehicle for FLU drug to the infected target cell, which is used to cure prostate cancer [6]. Based on DFT theory, the interaction and bond properties of anticancer drug doxorubicin (DOX), armchair single-walled carbon nanotube (SWCNT), and hydroxyl- and carboxylfunctionalized SWCNT (*f*-SWCNT) showed that hydrogen bonds between active sites of DOX molecules and hydroxyl- and carboxyl-functionalized CNTs played a more important role than those with pristine CNTs in the adsorption and fixation of the studied complexes as well as their thermodynamic energy [7]. The effect of ethanol as a cosolvent on the inclusion complex formation between Flutamide drug molecule and the carbon nanotube. The results reveals that the presence of ethanol at the concentration of 0.5 M enhances the stability of the simulation system. Taken altogether, the obtained data provide useful information about the ethanol co-solvent effects on the adsorption process [8].

Yoosefian et al. investigated the functionalized single-walled carbon nanotubes as a carrier for Droxidopa and observed more dispersibility of single-walled carbon nanotubes and improved bioavailability with reduced systemic toxicity [9]. The drug carrier, N-isopropyl acrylamide-Carbon nanotube is suitable for the delivery of Doxorubicin, and five mer N isopropyl acrylamide is the optimum carrier for Doxorubicin loading [10]. The effect of the functional group of nano-carrier on the drug binding was investigated by all-atom molecular dynamics (MD) simulations of anticancer drug, paclitaxel (PTX), loaded with the pristine SWCNT and functionalized with (-OH), (-COOH), and PW3

peptide shows the biological applications of single-walled carbon nanotubes (SWCNTs) including biomolecules carriers [11].

Kamel et al. have studied the drug delivery performance of the functionalized (5, 5) single-walled carbon nanotube with a carboxylic acid group for Flutamide anticancer drug in the gas phase and water solution by means of density functional theory calculations and obtained that the drug molecules are strongly adsorbed on the functionalized nanotube surface [12]. The Density functional theory calculations on the effects of covalently binding isoniazid, an antitubercular compound to functionalized carbon nanotubes and fullerenes clearly shows the solubility of functionalized carbon nanotubes is higher than functionalized fullerenes and the dissolutions in water are thermodynamically favourable [13]. In a study, the drug loading efficacy of graphitic carbon nitride (g-C3N4) for an anticancer drug, cisplatin was evaluated, the findings suggest that g-C3N4 could be used as an efficient drug-delivery system for the cisplatin drug to treat various types of cancer [14].

Table 1: Few examples of CNTs as Drug Delivery carrier

S. No.	Drug carrier	Drug	Disease	Reference
1.	Graphdiyne nanotube (Gdn-NT)	Flutamide (FLU)	Cure prostate cancer	V. Nagarajan *et al.*
2.	Armchair single-walled carbon nanotube (SWCNT) and hydroxyl-and carboxyl-functionalized SWCNT (*f*-SWCNT)	Doxorubicin (DOX)	Anticancer drug	Sina Karimzadeh *et al.*
3.	Single-walled carbon nanotube	Flutamide	Anticancer drug	Maedeh Kamel *et al.*
4.	Single-walled carbon nanotubes	Droxidopa	Orthostatic hypotension	Mehdi Yoosefian *et al.*
5.	N-isopropyl acrylamide-Carbon nanotube	Doxorubicin	Anticancer drug	Reza Maleki *et al.*
6.	Single-walled carbon nanotubes (SWCNTs)	Paclitaxel (PTX)	Anticancer drug	Leila Tohidifar *et al.*
7.	Single-walled carbon nanotube	Flutamide	Anticancer drug	Maedeh Kamel *et al.*
8.	Carbon nanotubes and fullerenes	Antitubercular compounds	Tuberculosis	Marco Gallo *et al.*
9.	Graphitic carbon nitride	Cisplatin	Anticancer drug	Mehvish Perveen *et al.*
10.	Pristine and B-, Al-, Ga-doped C36 nanotube	Fluorouracil	Anticancer drug	Mustafa Kurban *et al.*
11.	Single-walled carbon nanotubes:	Carmustine	Brain tumors	Rabeeh Khorram *et al.*
12.	Functionalized carbon nanotube	2-methylheptylisonicotinate	Antitubercular drug	Nabanita Saikia,
13.	TiO_2 NT, SiO_2 NT and CNT	Chitosan monomer		
14.	Carbon nanotube	Hydroxyurea	Anti-cancer drug	Maryam Hesabi *et al.*
15.	Pristine, Al-, and Si-doped carbon nanotubes	5-fluorouracil	Cancer drug	Mohammad Yahyavi *et al.*
16.	Carbon nanotube	Cladribine	Anticancer drug	Mina Lotfi *et al.*
17.	Graphdiyne nanotube (Gdn-NT)	Imuran (Azathioprine) Pentasa (Mesalazine) Hyoscyamine (Daturine)	Crohn's disease and rheumatoid arthritis Crohn's and other inflammatory diseases Parkinson's disease symptoms	U. Srimathi *et al.*
18.	Carbon nanotubes (CNTs)	Efavirenz (EFV)	anti-HIV drug	Hong Xu *et al.*

Density functional theory (DFT) is used to examine the formation possibility of a stable interaction between 5fluorouracil (5-FU) drug molecule and a pristine, boron (B), aluminum (Al) and gallium (Ga)-doped carbon nanotube (CNT), the observed result shows that Al-doped CNT has more desirable properties to use it as a drug delivery system [15]. The adsorption behavior of Carmustine drug on the surface of (5, 5) pristine single-walled carbon nanotube and the functionalized single-walled carbon nanotube with a carboxylic acid group is studied by density functional theory calculation, the result indicated that the Carmustine molecule can be adsorbed on the nanotube surface with a charge transfer from the nanotubes to drug molecule [16].

Carbon nanotubes can act as a suitable drug delivery vehicle for internalization of MHI within biological systems. The interaction of 2-methylheptylisonicotinate (MHI) drug with (5,5) armchair single-wall carbon nanotube (SWNT) of finite length is studied using density functional theory, the results are used to identify the potential applications of functionalized carbon nanotubes as drug delivery systems [17]. In a research work, theoretical studies on density functional theory (DFT) have performed to understand the interaction between the Chitosan (CS) monomer and three types of nanotubes, namely TiO2 nanotube (TiO2 NT), SiO2 nanotube (SiO2NT) and Carbon nanotube (CNT) [18].

The interaction of the anti-cancer drug hydroxyurea with carboxyl-functionalized zigzag carbon nanotubes (CNTs) studied by the method of the density functional theory (DFT) at B3LYP and CAM-B3LYP levels in gas and solvent phases, observed data indicates that adsorption is dependent on the carboxyl sites of the nanotube as well as on the sites of the drug, also the hydrogen-bonding interactions between drug and COOH-CNTs play an important role for the different kinds of adsorption observed [19].

Yahyavi et al. investigated the interaction between pristine and doped carbon nanotubes (CNTs), and 5-fluorouracil (5FU) using density functional theory (DFT) method and suggest that Al-doped CNTs is expected to have promising application in the field of drug delivery [20]. Lotfi et al. studied the pristine (NT) and COOH (FNT) functionalized carbon nanotube, ten noncovalent configurations and four mechanisms of covalent functionalization of NT and FNT with cladribine anticancer drug (CDA), the free energies of solvation shows that NT and FNT solubility increases in all drug-nanotube configurations which is a main factor for its applicability in the drug delivery [21].

The density functional theory calculations of adsorption of the drugs, Imuran (Azathioprine), on graphdiyne suggested that the graphdiyne nanotube can be effectively utilized as a drug delivery system for the chronic disease drugs [22]. Xu et al. studied the capability of the boron nitride nanotubes (BNNTs) and carbon nanotubes (CNTs) as the delivery vehicles of EFV, the results suggested that EFV can be adsorbed physically on the CNTs with a stable state, indicating that CNTs may be a potential delivery vehicle of EFV, the computed interaction energies reveal that the adsorption of EFV on CNTs are more favorable than that on BNNTs [23].

3. Conclusion

CNTs are promising nano-carriers for both drugs as well as biomolecules. This study possess in-depth knowledge and understanding of carbon nanotubes both for their pharmacotoxicological properties in drug molecule, it is essential to recommended for routine clinical use in the form of drug delivery carriers in the diagnosis and treatments of many diseases.

4. Future perspectives

The future research should be focus on investigating more efficient CNT based drug delivery for the betterment of human health. In addition, progress in carbon nanotube technology may well lead to better insights into biological and physical chemistry processes through theoretical calculations. This will make it possible to find drug molecules more compatible with carbon nanotube to facilitate in medical field.

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Some results on undamped force vibrations of a spring using numerical methods

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ABSTRACT

In this paper have been discussed the numerical technical solutions for some undamped force vibrations of a spring problem using well-known numerical methods such as Runge-Kutta fourth order classical method and Eulers Modified Method.

Keywords: *Undamped forces, differential equations, numerical methods*

1. Introduction

From last few decades considerable efforts have been made using some techniques towards the development of computational methods to solve numerically linear differential equations in various fields of science and engineering. The analysis was made in applied physical sciences. Some methods are applied to find the numerical solution of problems related to science and engineering. Now a day's numerical methods have been attracted the great interest towards researchers of physical and mathematical sciences and many research papers were published in these fields.

2. Undamped force of vibrations

(Forced undamped vibration is described as the kind of vibration in which a particular system encounters an outside force that makes the system vibrate). Examples of undamped forced vibration are: Movement of laundry machine due to asymmetry. The vibration of a moving transport due to its engine. Movements of strings in guitar.

Consider the undamped forced vibrations of spring given by the differential equation is

$$m\frac{d^2x}{dt^2} + kx(t) = f(t) \qquad \ldots (1)$$

In this paper we take the special choice of $f(t) = (1-\sin t)$, m=1kg, k=1N/m, with initial conditions $x(0) = x'(0) = 0$ then equation (1) gives us

$$\frac{d^2x}{dt^2} + x(t) = (1-\sin t),$$

As the initial conditions,

The exact solution of equation (1) by using the classical method is

$$x(t) = \frac{t^2}{2} + \sin t - \frac{xt^2}{2} + \frac{t}{2}$$

Applying initial conditions we get $C_1 = -1$, $C_2 = 0$.

3. Runge-Kutta Method

To compute for $y(x_0 + h)$ the required value of $y'(x_0 + h) = z(x_0 + h)$.

Firstly we compute the values of

$k_1 = hf(x_0, y_0, z_0)$; $l_1 = hg(x_0, y_0, z_0)$

$k_2 = hf\left(x_0 + h/2, y_0 + k_1/2, z_0 + l_1/2\right)$; $l_2 = hg\left(x_0 + h/2, y_0 + k_1/2, z_0 + l_1/2\right)$

$k_3 = hf\left(x_0 + h/2, y_0 + k_2/2, z_0 + l_2/2\right)$; $l_3 = hg\left(x_0 + h/2, y_0 + k_2/2, z_0 + l_2/2\right)$

$k_4 = hf\left(x_0 + h, y_0 + k_3, z_0 + l_3\right)$: $l_4 = hg(x_0 + h, y_0 + k_3, z_0 + l_3)$

$y(x_0 + h) = y_0 + 1/6\left(k_1 + 2k_2 + 2k_3 + k_4\right)$ and

$y'(x_0 + h) = z(x_0 + h) = z_0 + 1/6(l_1 + 2l_2 + 2l_3 + l_4)$

4. Eulers Modifeid Method of 2nd order

If h is the step size, Lets consider equation differential equation of (1)

$x'' = (1 - \sin t) - x(t)$ ... (2)

$\frac{dx}{dt} = z = f(t, z, x)$ then equation (1) reduces to

$\frac{dz}{dt} = (1 - \sin(t)) - x = g(t, z, x)$

Consider the Eulers approximation values as follows

$x_1 = x_0 + hf\left(t_0, z_0, x_0\right)$

$z_1 = z_0 + hg(t_0, z_0, x_0)$ and so on.....

Table 1: Results from Different numerical methods

h=1/32	Exact solution	Ruge Kutta Method x		Eulers Method	
t		t	Error	t	Error
1	1.2835	1.30891	0.42758	1.3005	0.43128
3	1.2568	1.74521	0.52969	1.72412	0.52712
5	2.0012	2.18151	0.53833	2.1717	0.52181
7	3.1258	3.05411	0.43125	3.0521	0.42181
9	2.8592	3.49041	0.47056	3.50125	0.42158
11	3.2561	4.36301	1.06535	4.32156	1.06421
13	3.1258	4.79932	1.6196	4.80012	1.62131
15	4.1258	5.23562	2.24149	5.28523	2.25863

5. Comparison of two numerical solutions

In this section, we compare the results of present method with classical method. In order to verify these techniques of two methods and classical methods have been selected for our results. For both the methods we taken step size as h=1/32 has been chosen and table 1 gives a data with respect to different solutions.

6. Conclusion

Here we have assumed and taken the equation of undamped forces of vibrations which are physically represented in the form of differential equation and hence solved classical method and also numerical method and discussed.

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