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RESEARCH ARTICLE

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Nanostructures and applications

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ABSTRACT

Nanotechnology is an interdisciplinary area that studies materials and structures of billionths in size and their uses. Nanomaterials are the keystones of nanotechnology and have exclusive electrical, magnetic and optical properties. What makes nanotechnology so stimulating is that materials perform contrarily in this dimension than in the macro world. The weight/power proportion, magnetic and optical possessions as well as conductivity alter meaningfully as you change from the macro dimension to the nano dimension. In this investigation, after giving overall data about nanomaterials, nanosystems, nanomachines, nanorobots and nanosystems from nanostructures were examined. Then, from nanostructure applications to the automotive industry, energy. defense and environmental applications were examined. Finally, nanofuture for nanostructures is discussed.

1. INTRODUCTION

Nanotechnology is the control and engineering of technical consequences subsequent from the appearance of new possessions of substance at the nanoscale (billionth of a meter). Nanoscale is an approximate material scope. At the nano level, the chemical, biological and physical properties of matter vary essentially and expressively. There are fundamental variations in the possessions of separate atoms, molecules and mass.

About arrangement, nanomaterials have tremendously trivial dimensions and as a minimum one dimension is 100 nm or smaller. Nanomaterials can be nanoscale in one, two or three dimensions. They can be found in single, fused, clustered or clustered forms with tubular, spherical and uneven forms [1]. Communal kinds of nanomaterials comprise fullerenes, nanotubes and quantum dots. Nanomaterials have uses in the area of Nanotechnology and show dissimilar physical chemical properties from normal chemicals such as Silver Nano, Fullerene and Silica) [2].

Perspectives on nanostructures essential to encompass the insights and boundaries of numerous systematic disciplines. It has been stated that the benefit of nanostructures will be its application in catalysis, but the chemist is also investigating nanoscale materials and must ensure that quantum detention effects are displayed. Nanometer-sized materials are best articulated in optical or electronic technology, where the nanostructure can be insulated from the molecules encountering, thus avoiding any chemistry risks [3].

The aim of this study is to critically examine nanostructures and their applications. Within nanostructures, nanomachines, nanorobots as well as nanosensors have been explained and critically discussed. Then, nanostructure applications in the automotive industry, energy, defense and environmental fields are systematically explained, and finally, a future-oriented perspective on nanostructure is given to motivate young generations to research and to point out the deficiencies in the related field of study.

2. NANOSTRUCTURES

Nanostructures are synthetic and are structures ranging from 1 nm to 100 nm. Nanostructures can

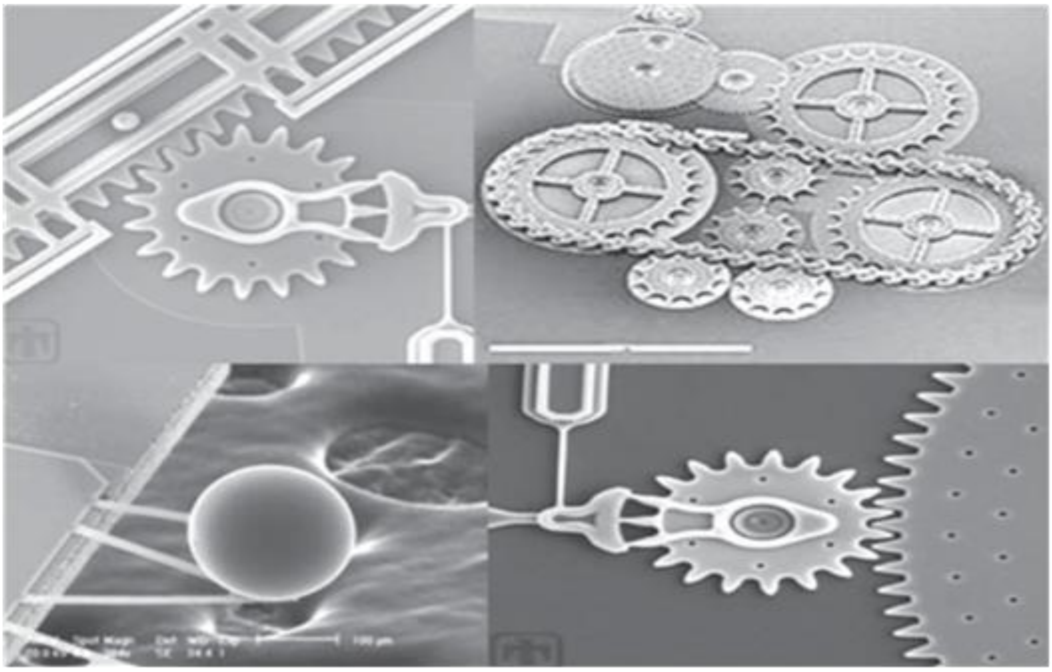

Figure 1. Various examples of gear wheels and motor components at the nanoscale [4]

be designed according to a wide variety of physical properties such as nanosurfaces and cylindrical nanotubes.

2.1. Nano-machines

Nanomachines, the smallest of which are the size of a virus, are much lesser than a human cell, often dignified in micrometers (millionths of a meter). Investigators turned to natural biological technology for motivation when emerging nanorobots because most robotic construction techniques at this scale would be impossible. We previously have billions of organic nanobots within us powering many functions of our cells. For instance, ribosomes are organic nanoscale forms of organic devices. The nanites are not your typical mechanical robots. They are not made of metals that come to attention when you think of a robot. As an alternative, nanomachines are constructed from DNA or other biological substances that flawlessly interrelate with biological surroundings in certain ways to achieve specific results.

The microscopic size of nanomachines means high working velocity. This is an outcome of the natural propensity of all machines to run faster as they get smaller in size. Nanomachines can be programmed to work synergistically to replicate themselves or create larger machines or nanochips. Particular nanomachines named nanorobots could be designed to not only identify but also treat illness states, maybe by finding and destroying occupying bacteria and viruses. In Figure 1, several examples of gear wheels and motor components at the nanoscale are given.

Additional benefit of nanomachines is that the individual units need very little energy to work. Resilience is extra potential advantage; nanites can last for centuries before deteriorating. The main difficulty lies in the production methods. It has been recommended that some nanomachines could be grown in a manner alike to how plants change from seeds.

Medicine is continually developing and new technologies are constantly being incorporated into the diagnosis and treatment of patients. Numerous nanomachines and other nanoobjects presently under study in medical investigation and diagnostics will soon find application in medical practice [5].

The biological and physical disciplines have a mutual attention in minor constructions. For the physical sciences, "nano" proposes quantum phenomena and extraordinary physical possessions. Biology enhances extremely advanced nanomachines that work completely with

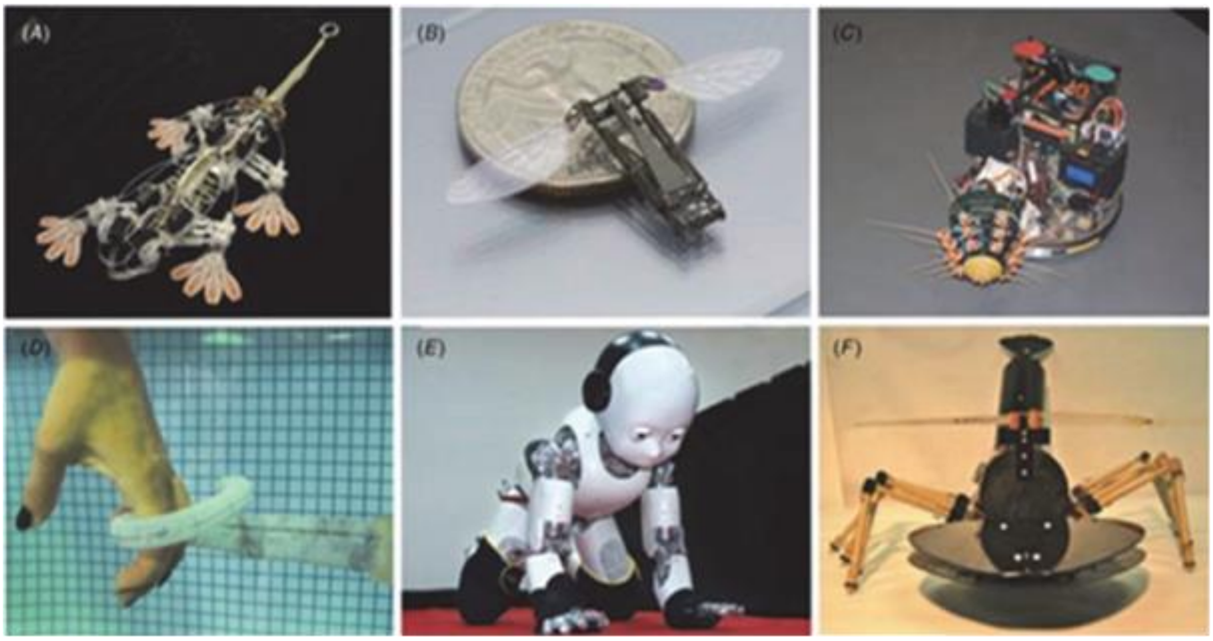

Figure 2. Examples of microrobotics inspired by Bio Organisms [4].

classical molecular mechanisms. To the biological disciplines, "nano" suggests a new framework—from most physical disciplines—on which to hang thoughts about new tools and useful sets that will be needed to assemble an intangible model of life [6].

2.2. Nano-machines

Nanorobotics is one of the most important technology areas of the last period. It can be characterized as the design, development and manufacture of nano/micro scale machines by using robot systems or components at nanometer scale and/or approximate sizes.

Nanorobotics is the engineering discipline that includes the design and construction of nanorobots. It covers the construction of devices, tools and systems with nanoscale components or molecular components in 0.1-10 micron sizes.

In this field, besides "nanorobots", there are also denominations such as "nanobots", "nanoids", "nanites", "nanomachines" or "nanomites". In Figure 2, illustrations of microrobotics inspired by Bio Organisms are shown.

"Nanorobots", the first applications of which began to be seen in the field of medicine and health, can be defined as nanoassemblies that protect the human body against pathogens and keep it in balance.

Their approximate diameter is designed to be around 0.5-3 microns. Intensive research programs are carried out on nanorobots, whose components, parts and sub-mechanisms are planned to be 1-100 nanometers in size.

Nanorobotics enable controlled operation of schemes at the nanometer scale. The ability and behavior of cooperating in sync with the algorithms and control methods put on individual robots is described as "swarm behavior", just like in bees and ants. With these algorithms, it is possible to control the collective movements of hundreds or even thousands of robots. In Figure 3, similar "hive behavior" is of great importance in nanorobots, just as the synchronized movement of bees around a hive.

Small doses of drugs or chemicals can be carried in a suitable chamber on the nanorobots. The nanorobot can release the drug directly into the diseased area or wound. Nanorobots can also be used directly in cancer treatment by carrying chemotherapy chemicals. Smaller amounts of drugs/chemicals that can be secreted directly onto the cancerous tumor will be more effective than conventional chemotherapy treatment.

Figure 3. Similar "hive behavior" is of great importance in nanorobots, just as the synchronized movement of bees around a hive [4].

Within the Probe, Knives and Chisels, Lime is used for cutting out clots and obstacles. At the same time, equipment is needed to break up the clots into small pieces.

Also known as bionanorobotics, this field deals with nanorobots inspired directly from biological organisms. In bionanorobotics, the dimensions are at the micrometer level, and they are formed by using and mounting nanoscale components in these systems on a large scale. The main topics covered in bionanorobotics can be classified as design, construction, programming and control.

Based on this, nanorobots represent an integrated integrity that includes systems with actuation, sensing, signal processing (transmission-reception), information processing, intelligent and/or hive behavior capabilities.

Some of the main purposes targeted with nanorobots can be listed as follows:

Cloning of organs and their use for change in diseased bodies;

Repairing skin cells that cause aging with nanorobots placed in the body; meanwhile, it is also aimed to repair diseased cells or organs.

In this process, nanorobots will be able to develop new chemical compounds and building-building materials and create new electronic components.

They will be able to transform the substance for food purposes. As a result, it will be possible to cope with hunger and diseases on earth.

The ozone layer can also be used effectively to eliminate environmental problems, especially global warming problems.

In the medical field, nanorobots are considered to be designed to perform a wide range of tasks, such as diagnosis, monitoring and treatment of deadly diseases:

- Drug Release (drug delivery)
- In-house Tracking-Tracking
- Dentistry
- Cancer Detection and Treatment
- Diagnosis and Treatment of Diabetes
- Precision Surgeries
- Gene Therapy

These nanorobots deliver drugs or chemicals to specific target areas within the human body.

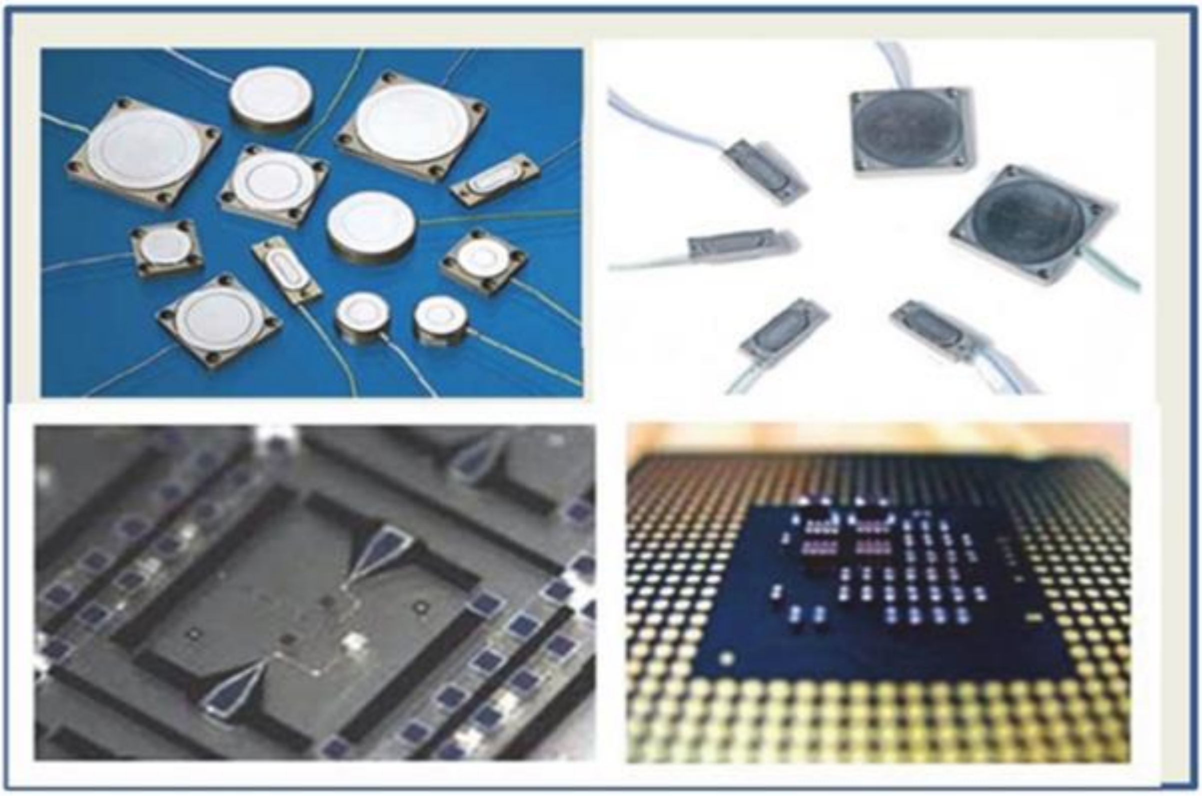

Figure 4. Various types of nanosensors.

2.3. Nano-sensors

The nanosensor transforms the data and information obtained from the atomic scale and nanoparticles into analyzable macro scales. Its biggest advantage is that it can work in small places that macro- and micro-sensors cannot reach; require less power in their operation; higher precision and adaptability for specific purposes. In Figure 4, numerous types of nanosensors are illustrated.

Nanosensors are devices and mechanisms that are nanoscale (one billionth of a meter), extremely small in size and capable of detecting and diagnosing physical stimuli (stimuli). These physical warnings can be listed as follows: chemical and biological substances, movement, mass, acoustic, force, force, electromagnetic, thermal-heated.

Application areas of nanosensors are as follows: Medicine, pharmaceuticals, health technologies, ecology, environment, security, defense and military, industrial, aerospace, daily life, white goods, transport, communication, integrated circuits, building and facilities. Recently new investigations have been reported on drug delivery [7] and sensor applications [8] to detect disease site and cure it with appropriate drug delivery application.

In addition to the progress reached in biosensor technology, fully automatic, real-time, high-sensitivity, label-free and multilayer biomolecular detection and diagnostic sensors have brought important applications with the advantage of nanotechnological developments. Thus, with these technologies, the possibility of early diagnosis of all possible abnormal data has emerged with routine health checks at home. In Figure 5, In_2O_3 nanowire based nano biosensors are displayed.

3. APPLICATIONS

Nanostructures can be applied in many places. In this part, few of them including automotive industry, energy, defense as well as environmental applications will be described.

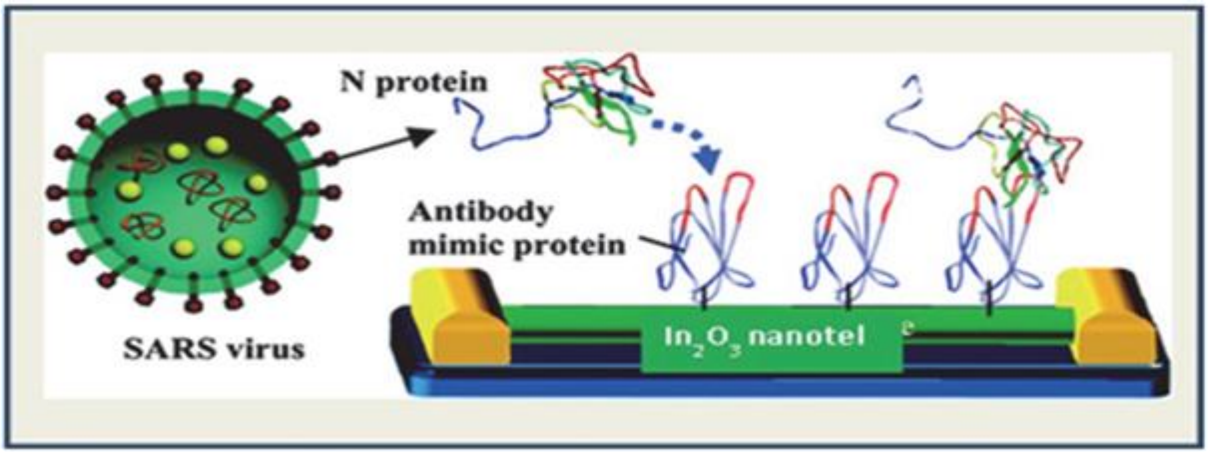

Figure 5. In_2O_3 nanowire based nano biosensors.

3.1. Automotive industry

Nano-structured substances, one of the most significant zones of nanotechnology, are of countless significance for the car production.

Initially, besides vehicle safety and security, nanomaterials will play a serious part in struggles to decrease automobile mass, advanced strength and more flexible constructions.

Steel is the most significant structural material utilized in vehicle bodies in the automotive production.

The utilize of high-strength steels in car bodies is being investigated. Nevertheless, there are deviations in the shaping of the steel in the cold state, in the dimensioning of the car frame.

This issue was tried to be overwhelmed with hot forming. Though, due to the high temperature, there is a problematic of scale creation on the surface.

Here, this can be eliminated with a multifunctional coating on the surface with nanotechnology. Glued and linked nanosized glassy substances together with aluminum form a robust layer on the surface.

With nanotechnology, scratch-resistant, dirt-proof and self-repairing car paints can be smeared on the vehicle external.

This is done with nanoparticles in the nanocoating technique, with layers that are flexible, fast-adhesive, corrosion-resistant and antimicrobial.

Amongst the systems shown in the figure on the other page, anti-fogging, antifungal, anti-reflective coatings are also flattering extensive thanks to nanotechnologies.

3.2. Energy

World-wide energy wants are fossil-based fuels, which are supplied equal to about 210 million barrels per day. 85 million barrels of this is delivered by oil (40%). At this point, the quantity of renewable energy is little. It is unspoken that this state will increase slowly when the world's energy needs are taken into account, and the associated CO_2 release to the atmosphere will reach alarming proportions.

With pyroelectric ZnO nanowires, in the change founded on temperature change, time-dependent temperature alterations can be converted into electricity with impulsive polarization. This energy change takes place with the semiconductor and pyroelectric properties of ZnO. The nanogenerator advanced here is balanced and will be able to encounter the energy supplies of nano expedients by changing waste energy.

Nanotechnologies have countless potential for cleanser, effectual and ecologically kindly energy production. Energy-related technologies in which nanotechnologies can play significant roles are given as follows: heating, lighting, convection, renewable energy, fuel cells, energy storage, hydrogen production and storage. Nanostructures

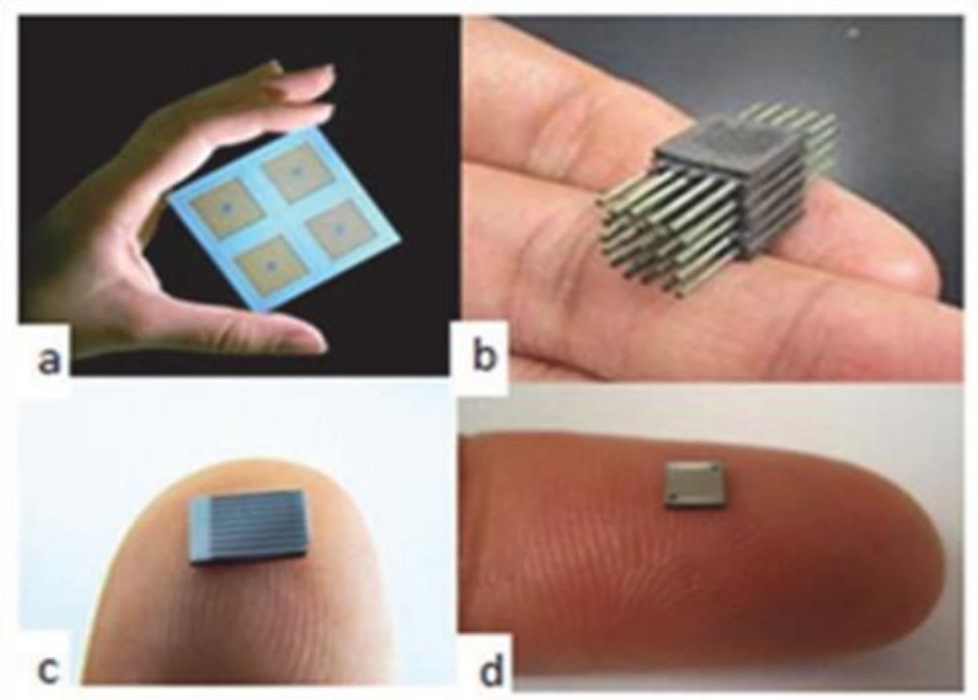

Figure 6. New generation fuel cells with nanotechnology applications.

are recently used in energy conversion and storage applications [9].

Nanofluids are shaped by mixing the CNTs added into the water. With the heat transfer of nanofluids, 10% higher efficacy can be attained in central heating schemes.

Contingent on the substances in the fuels, more efficient energy use is possible with nanotechnology. Additional effectual batteries and accumulators can be advanced with lighter and stronger materials. With such materials, an important upsurge in efficacy and success can be achieved in the conveyance industry. Here,

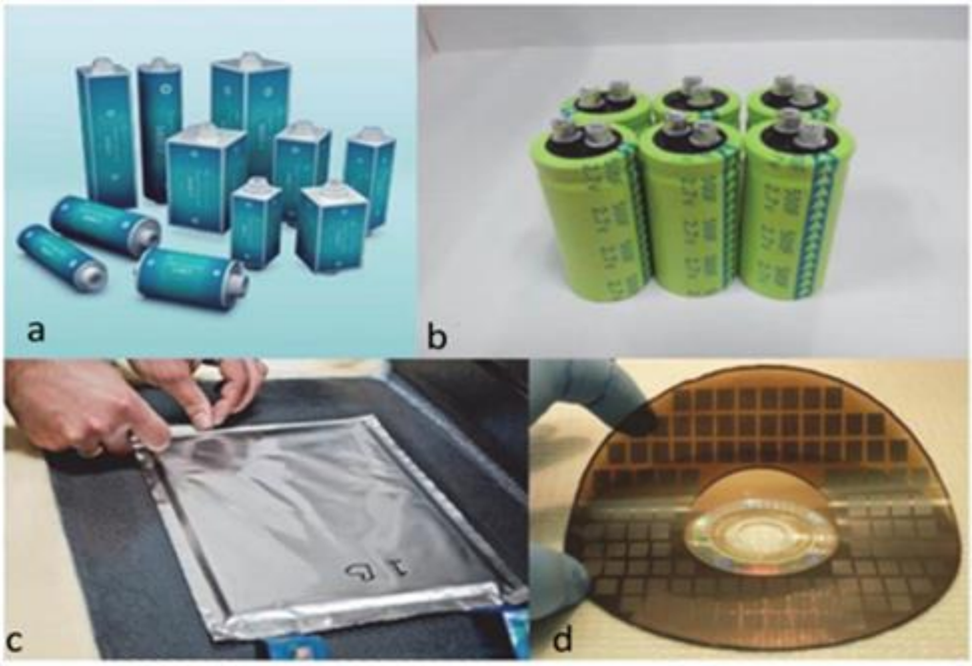

Figure 7. Various battery and energy storage examples with nanotechnology.

lightness and durability are especially significant for more effectual energy usage. In Figure 6, fuel cell applications and in Figure 7, battery and energy storage examples are shown. Selenium semiconductor structures are used in energy storage area such as rechargeable batteries [10]. Also, solar and thermal energy conversion expedients are applied for outdated photovoltaic, solar thermal, and solar thermo-photovoltaic expedients [11].

3.3. Defense

Nanotechnological progresses have led to the appearance of textile goods that have significant purposes in textile science and machineries. Combat uniforms with the subsequent features and qualities, with nanotechnological developments that can meet the necessities anticipated from uniforms and war clothes for defense technologies, camouflage covers and nets, clothes were industrialized.

Today, Unmanned Aerial Vehicles are extensively utilized for both observation and attack and annihilation purposes. Different mini-vehicles are being developed for military units and special units, marching, flying and naval at the micron level for even smaller and instantaneous short-range and short-range reconnaissance and observation. Observation tools containing different land-air-sea nanocomponents for reconnaissance-observation purposes are shown in Figure 8.

It is perceived that numerous novelties in nanosciences and nanotechnology have started to be implemented in land, air, sea and space vehicles, which are the most planned zones in defense fields. Defense vehicles all over the world are flattering zones where nanotechnology is utilized in every feature as progressive technology stages in a tremendously diverse and wide range. The illustration on the other page shows the defense utensils wherein dissimilar nanotechnologies are smeared and which attract attention particularly with their "stealth" structures. The latest warplanes, helicopters and war boats and warships developed with ghost stealth structures are exposed in Figure 9.

Nanosciences and nanotechnological innovations have started to be used in areas involving the security of society as well as military areas. Especially in the period following the September 11 attacks in the USA, there have been important developments in the concept of "homeland security" in terms of providing the highest level of security with advanced technological opportunities and capabilities.

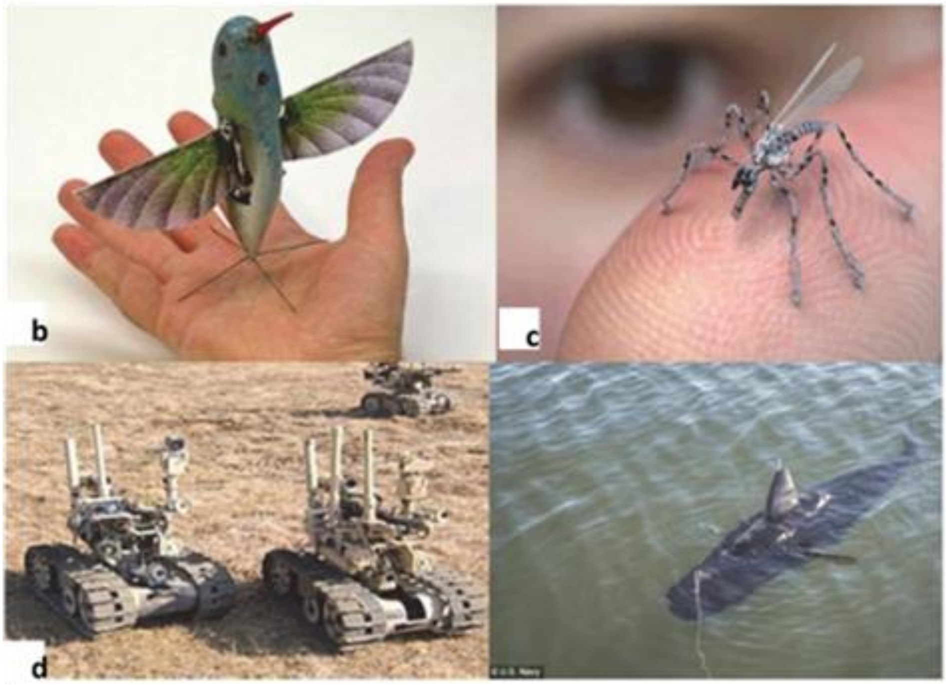

Figure 8. Observation tools containing different land-air-sea nanocomponents for reconnaissance-observation purposes.

Figure 9. The latest warplanes, helicopters and war boats and warships developed with ghost stealth features.

For the first time in the early 90s, the University of California, USA, Prof. Dr. In the "smart dust" technology introduced by Pister, the aim is to reduce the dust, grain (rice grain size), small stone-sized platforms to extraordinarily small (nano) sizes for the purpose of collecting, evaluating and transmitting news and data anytime, anywhere, to create a highly effective security network. aims to establish. The first examples are the size of a matchbox and capable of continuous data communication (including video images) from a distance of approximately 13-15 km, and they are placed in cities, on lands, in the atmosphere, and used for observation-exploration and monitoring purposes.

3.4. Environment

Nanosensor applications that can unceasingly measure air, water and environment pollution and give warning and alarm in case of nonconformity from the given threshold values are becoming

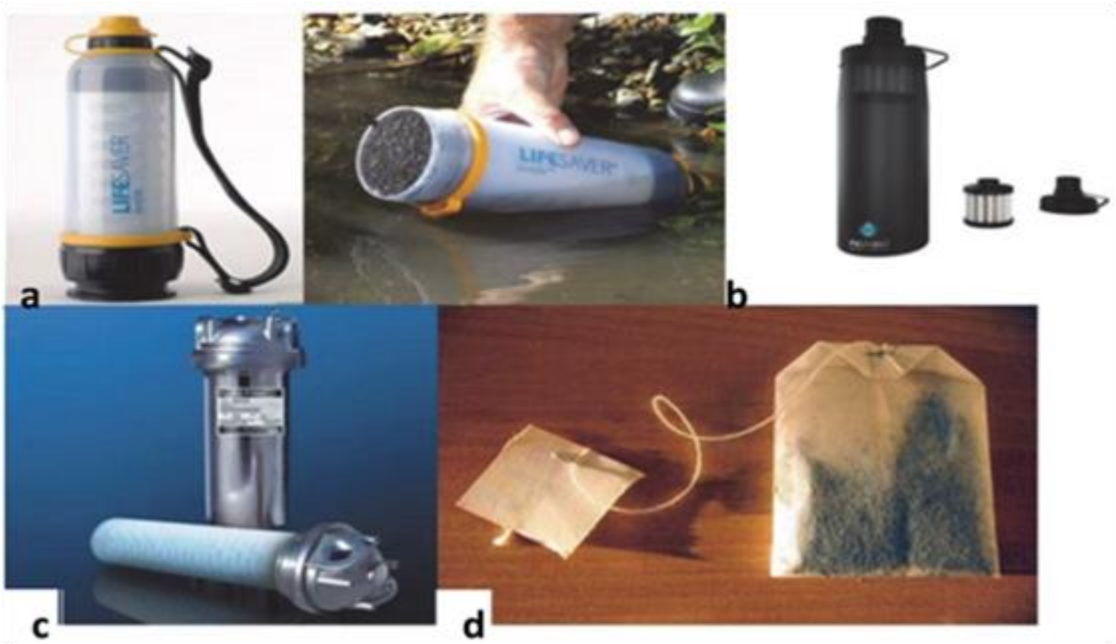

Figure 10. Nanotechnological water purification, filtering and purification application examples.

Figure 11. Airgel and silica-airgel specimens that can efficiently spotless against water, sea-ocean, and ground oil spills.

widespread. Nanosensors have a crucial part in observing the ecological quality of air, water and environment with full and sensitive data. Different nano-structured materials have been advanced for the discovery of dissimilar mechanisms.

Potable, clean water is one of the most important needs of almost every society and is often limited. It has been determined that approximately 780 million people have significant problems in accessing drinking and clean water resources. It is of great importance to develop innovative, inexpensive and practical methods with nanotechnology against the known possibilities of obtaining drinking water from sea water. Examples of nanotechnological water purification, filtration and purification applications are shown in Figure 10.

Environmental cleaning (remediation) consists of parting and other procedures, as well as works that are free from chemical and radiological pollutants and will not imperil human health. With nanomaterial applications, quicker and more cost-effective spring-cleaning and cleansing is possible. The most suitable method in nanotechnological approaches is discrimination and cleaning and removal of organic/inorganic contaminants. In Figure 11, airgel and silica-airgel samples are shown that that can efficiently spotless against water, sea-ocean, and ground oil spills.

3.5. Others

Silicon carbide [12], peptide [13] and hybrid [14] nanostructures have been reported in the use of biomedical applications, respectively. Also, self-assembled [15] and aptameric-functional DNA structures [16] are reported to use in biomedical and biological applications, respectively. Furthermore, copper sulfide nanostructures are investigated and reported the outcomes. CuxSy nanostructures are talented materials for both detecting and bio-imaging requests [17]. The usage of CuxSy NPs is not restricted to cancer, but can also be utilized in the treatment of many in vitro antibacterial diseases. This review mainly focused on the synthesis, properties and applications of CuxSy nanostructures as biosensors and their usage in cancer analysis and treatment.

4. FUTURE PERSPECTIVE

Although it is science-fiction, human beings have always wondered about the future based on their imagination. The general view of the world that will be shaped in the future as a foresight or foresight other than prophecy has been the subject of many studies graphically. Figure 12 shows the rapid

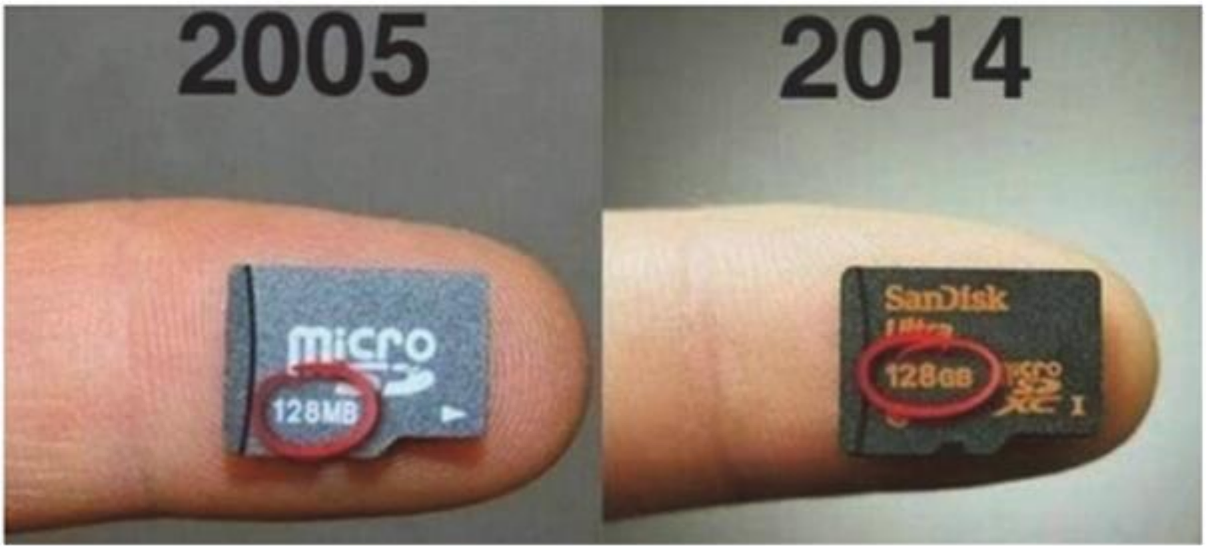

Figure 12. The development of flash drives is very fast: 128 MB capacity in 2005, 128 GB in 2014, 1 TB in 2020.

evolution of flash drives from 128 MB capacity in 2005 to 1 TB in 2020.

Cities of the future are expected as follows:

a. Astronomically high skyscrapers in cities with population growth; "megacities",

b. Due to the increasing traffic density, transportation must be made from the air at short distances; flying automobiles or transportation vehicles;

c. The absolute representation of the green image as a cause for concern; “green cities” where a more environmentally friendly and sustainable environment is created;

d. Undoubtedly, providing the energy source with non-polluting, recyclable and environment-friendly technologies;

e. The unavoidable pace of everyday life, ever increasing;

f. Cities built on mobile platforms or on water-sea or submarine/underground.

The vehicles of the future are expected to:

- Self-driving cars (Google has such a tool) and smart highways;
- Flying cars; anti-gravity devices;
- Flying, turbo and wheeled boats;
- Smart vehicles that are sensitive to the environment and can respond to different conditions;
- Electric vehicles that do not require charging; “solar” cars powered by solar cells.

Undoubtedly, humanity wants to see an environment of peace, a peaceful and war-free world in their dreams for the future. In general, various innovations and technologies awaiting the society of the future are listed below: the digital currency era; disappearance of cash; making "transhuman" (robocop!) with improvements in the human-machine interface; placement of implants in the body for identification, follow-up, monitoring; the aging of generations with the prolongation of life expectancy.

The following technological predictions are in question in the developments in medicine, health and life sciences that will affect the lives of individuals in the future world: average life expectancy above 100 years; healing of all kinds of diseases by DNA repair and manipulation; organ regeneration; designed dolls, bodies, organs; immediate pain relief, artificial muscles for maximum empowerment. In Figure 13, some possible examples of future medicine and health technologies are displayed.

A rapidly changing “Nano World” with developments, innovations and new discoveries in nanosciences and nanotechnology may take shape in our future. It is calculated that nanotechnologies, together with their key roles and rapidly combining with information-communication, biology and cognitive (brain and perception) sciences, will create vast innovation opportunities in all other science and technology fields.

Figure 13. Examples of future medicine and health technologies.

5. CONCLUSIONS

The subsequent deductions can be drawn from the current investigation:

a. Nanotechnology uses the results from the emergence of new properties of matter at the nanoscale. At the nano level, the chemical and physical properties of matter differ considerably. Nanosensors, Nanomachines and nanorobots are important systems used in nanostructures.

b. Nanomachines, the smallest of which are the magnitude of a virus, are much lesser than a human cell and are usually measured in micrometres. There are already billions of organic nanobots within us that power many functions of our cells. Nanomachines are fabricated from DNA or other biological materials that flawlessly interrelate with biological environments in certain ways to achieve specific results. One benefit of nanomachines is that the separate units involve very little energy to operate. For example, nanites can last for periods before deteriorating. The chief difficulty lies in the production approaches.

c. "Nanobots", the first applications of which began to be seen in the field of medicine and health, can be defined as nano-mechanisms that protect the human body against pathogens and keep it in balance. Small doses of drugs or chemicals can be transported on nanorobots in a suitable chamber. The nanorobot can deliver the drug directly to the diseased area or wound. Nanorobots can also be used directly in cancer treatment by carrying chemotherapy chemicals.

d. The nanosensor transforms data and information from the atomic scale and nanoparticles into analyzable macroscales. Its biggest advantage is that it can work in small places where macro and micro sensors cannot reach; require less power in their operation; higher precision and adaptability for specific purposes. Application areas of nanosensors are as follows: Medicine, medicine, health technologies, Ecology, environment, Security, defense and military, Industrial, aviation, Daily life, white goods, Transportation, Communication, integrated circuits, buildings and facilities.

e. Nano-structured materials are of great importance for the automotive industry with their reduction in vehicle weight and their more flexible and durable structures. In addition, with nanotechnology, anti-scratch, dirt-proof and self-healing vehicle paints can be applied to the outer surface of the vehicle.

f. For the world's increasing energy needs, nanotechnologies have great potential for cleaner, efficient and environmentally friendly energy production. Among the important energy technologies in which nanotechnology can play a role, we can count heating, lighting, energy storage, hydrogen production and storage, and fuel cells.

g. Nanotechnological developments, combat uniforms that can encounter the necessities anticipated from uniforms and war clothes, camouflage covers for defense technologies have been established. Today, Unmanned Aerial Vehicles are extensively utilized for both surveillance and attack and destruction purposes. Different mini vehicles are being developed for military units and special units, flying, walking and at sea at micron level for smaller and instant short-range observation.

h. Nanosensors, which have become widespread recently, have an indispensable role in monitoring the ecological quality of air, water and the environment with full and sensitive data. Different nanostructured materials have been developed for the detection of different components. Faster and more cost-effective cleaning and purification is possible with nanomaterial applications. The most appropriate approach in nanotechnological methods is selectivity and cleaning and removal of pollutants.

i. There are the following technological predictions in the developments in medicine, health and life sciences that will affect the lives of individuals in the future world: the average life expectancy is over 100 years; Healing all kinds of diseases by DNA repair and manipulation; organ regeneration; designed babies, bodies, organs; instant pain relief, artificial muscles for maximum strengthening. In our future, a rapidly changing “Nano World” may be shaped by developments, innovations and new discoveries in nanoscience and nanotechnology. It is calculated that nanotechnologies will rapidly combine with information-communication, biology and cognitive (brain and perception) sciences with their key roles and create enormous innovation opportunities in all other science and technology fields.

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RESEARCH ARTICLE

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The effects of black tea extracts on the corrosion inhibition of mild steel in acidic solution

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ABSTRACT

It was examined to evaluate the effectiveness of extracted tea leaves as the green corrosion inhibitor that contains mild steel in acidic solvents. The test specimens were dissolved in an acidic solution with different concentrations of the extracted tea leaves. After 3 hours of immersion, the corrosion rate (CR) was measured. The results showed that a concentration of 1000 mg/l caused a significant inhibition in corrosion rate as compared to control. To see how black tea (BT) extract affected mild steel corrosion in 1 M HCl, it was subjected to a loss of weight procedure. The corrosion level and the inhibitor's performance were examined at five different BT extract concentrations, including 0.4, 1, 1.4, 2, and 2.4 g/l. According to the findings, increased BT concentration at every temperature decreased CR. As a result of the rise in kinetic activities of the metal surface interface, typically, temperature elevation leads to an increase in CR at every concentration of BT extract. The study's findings showed that adding 2.4 g/l of inhibition efficiency resulted in a temperature of 323 K, resulting in 84.95% inhibition efficiency. The small activation energy (Ea) of 8.74 and 11.45 kJ/mole reflected the barrier layer properties of BT extract and its chemical interactions on mild steel surfaces. The thermodynamic parameter revealed the spontaneous interaction between BT extract species and steel surface as k_{ad} rose from 0.929 to 1.728 $(g/l)^{-1}$.

1. INTRODUCTION

Metallic equipment corrosion has always been the biggest challenge in any manufacturing industry. The metal component exposed to a corrosive environment attack may impact the performance of the overall process [1]. Steel is considered one of the most popular alloys used extensively in mechanical equipment and industries like heat exchangers, boilers, and pipelines. The degradation of metal results in economic costs and could cause plants to shut down due to the harmful effect of corrosion on the product quality [2]. Many industries and operations use highly acidic media, especially HCl [3]. Acidity conditions may decline the equipment's service life; therefore, various corrosion control and monitoring techniques are used to prevent component failure [2-4]. Corrosion inhibitors are an essential method commonly used in aggressive environments to reduce, slow down, or delay corrosion of the components [5]. The dosage of the chemical substance should be in a specified treatment to work as an inhibitor, which could significantly improve the corrosion resistance and is considered a good protection technique for mild steel in various acidic solutions [6]. Chemical inhibitors are either inorganic or organic compounds. As the literature describes, most effective inorganic inhibitors like the sodium salts of chromate, molybdate, and others naturally form a passivation film due to oxidation [4]. These inhibitors, which accumulate on the metal surface and create a barrier film, primarily comprise oxygen, sulfur, nitrogen, alkenes, and phosphorous.

They are costly, dangerous, and may have devastating consequences for the ecosystem and physical health regarding chemical inhibitors. Green corrosion inhibitors have become popular recently because they are naturally safe, biodegradable, cost-effective, accessible, and free of harmful chemicals [7-9]. Various researchers have explored chemical inhibitors such as ferrous sulfate treatment [10], coating [11], and seeds and leaves of plant extracts [12-17]. It was found that green inhibitors could successfully reduce the corrosion rate and impede the growth of various microorganisms and fungi. Previous studies using natural inhibitors have shown that high levels of extract concentration do not affect eliminating corrosion. Thus, the black tea extract is applied as a green inhibitor to protect mild steel against corrosion in an acid solution by measuring the rate of metal removal at different temperatures and low concentrations of black tea extract from (0.4 to 2.4) g/l. The current approach includes the calculation of the kinetics and thermodynamics parameters with and without using inhibitors.

2. EXPERIMENTAL WORK

2.1. Mild steel specimens and solution preparation

A mild steel plate was cut in half to create a standard 30 x 20 x 2 mm size. The findings were pulverized using silicon carbide abrasive paper of (320-1000) grades for the oxide film to be removed. After that, the specimens were cleaned with water, polished, acetone-dried, and kept at 25 degrees Celsius for weight loss checks. Also, aggressive solutions of 1 M hydraulic acid were produced by diluting 37% HCl with distilled water and used as electrolytes for measurements.

2.2. Preparation of BT solutions extract

The packaged tea was bought at a nearby market and used to make black tea. The solution of BT extract was prepared by an aqueous solvent technique. 6 grams of BT was dissolved in 800 milliliters of boiling distilled water for exactly 90 minutes. The extract solution was then filtered and concentrated under a vacuum at 40 degrees Celsius for two hours. The 40ml extract was stored in the refrigerator for future use.

2.3. Weight loss measurements

An appropriate technique to assess corrosion is the analysis of loss of weight. A succession of emery papers was ground with mild steel coupons, then cleaned with acetone and dried at 25 degrees Celsius. The items were then weighed and put in a hundred milliliters of HCl, in the presence and absence of BT extract of different concentrations. A thermostatically regulated water bath was utilized to provide a steady temperature during the research at 293, 303, 313, 323, and 333 K. After three hours, the specimens were extracted and tested again using distilled water. Weight loss data was applied to determine the metal removal rate with Equation 1. [18].

$$CR\ (mm/y) = (87.6\ W)/D.A.T \quad (1)$$

One mm/y denotes 39.37 mpy, and CR represents the rate of corrosion in millimeters/year. W represents mg of weight loss, A reflects the whole opened surface area of the coupon in cm^2, T refers to the time of immersion (hours), and D equals 7.86 g/cm^3 is the specimen density.
Inhibition efficiencies (IE %) were computed from Equation (2) [19].

$$IE\% = \frac{CRo}{CRo - CR_{inh}} \quad (2)$$

Whereas CR_o, CR_{inh} are the corrosion rates in the absence and the presence of an inhibitor.

3. RESULTS AND DISCUSSION

3.1. The rate of corrosion

Table 1. The corrosion parameters were examined with and without different black tea extract concentrations levels after the weight loss was measured in 1 M Hydrochloric acid at different temperature.

BT extract concentration (g/l)	Temperature (K)									
	293		303		313		323		333	
	CR (mm/y)	IE%	CR (mm/y)	IE%	CR (mm/y)	IE%	CR (mm/y)	IE%	CR (mm/y)	IE%
Blank	19.33	-	23.52	-	30.22	-	36.01	-	40.22	-
0.4	12.50	35.33	14.24	39.47	15.35	49.22	16.68	53.66	19.84	50.66
1	11.05	42.82	12.08	48.62	13.40	55.64	15.69	56.42	18.42	54.20
1.4	8.79	54.52	10.50	55.34	10.99	63.62	11.66	67.61	15.96	60.31
2	6.67	65.49	7.24	69.20	8.39	72.23	9.27	74.25	11.95	70.27
2.4	4.33	77.56	4.68	80.08	5.25	82.61	5.41	84.95	8.24	79.51

The explanatory information is listed in Table 1. The CR measured was reduced due to the BT extract concentration increased at all temperatures. For example, the CR fell from 19.33 to 12.50 mm/y when 0.4 g/l BT extract was added to an empty acidic solution at 293 K. Also, in these experiments, the CR was clearly shown to be about five times less than in the use of 2.4 g/l BT. In addition, at all checked temperatures, the corrosion rate declines as the BT extract inhibitor concentration improves. As the BT concentration increases, the corrosion rate drops even at 293 K. In other words, when BT extract is introduced into an acidic solution to inhibit the corrosion process (to lower CR), it increases the protective effects on a steel surface. This confirms that BT extract has antimicrobial activity against various microorganisms and exerts a protective effect on metal surfaces [20]. In addition, when BT extract was present, a significant decline in CR was seen at elevated temperatures. The obtained results confirm the extract's 323 K high-temperature stabilities. This may be due to the high-temperature stability of the BT matrix [21], which resists degradation or interaction with other substances in the solution.

3.2. The inhibition efficiency

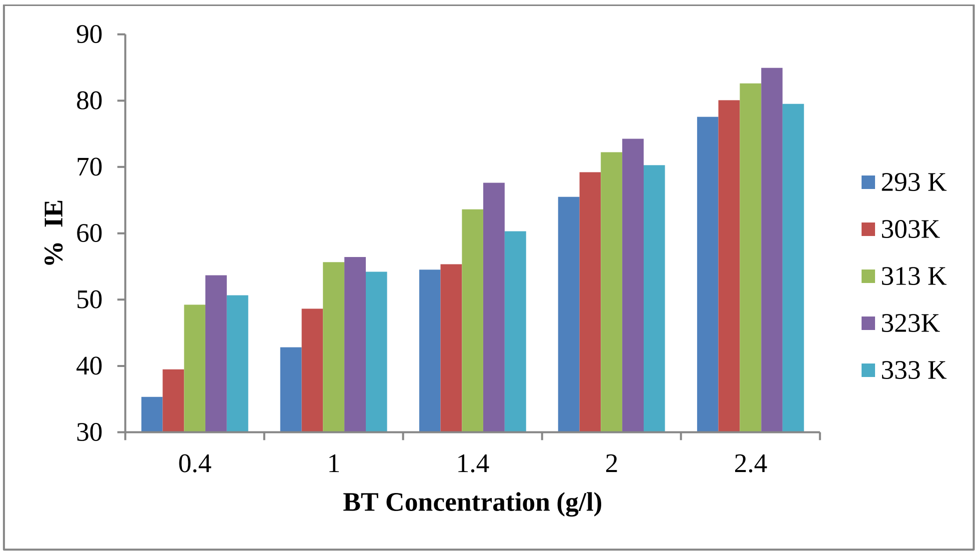

Figure 1. Variation of IE percentage with various BT concentrations and temperatures.

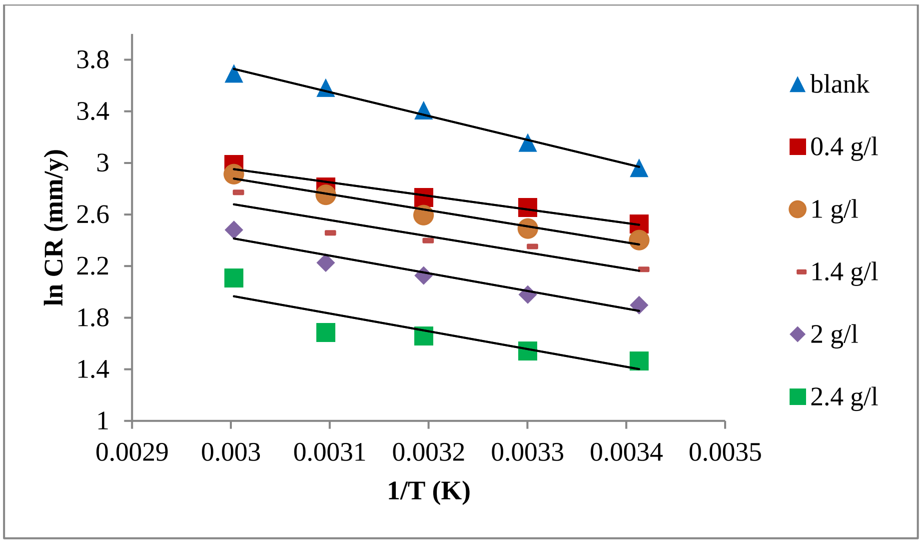

Figure 2. The Arrhenius plots of mild steel corrosion, alone and with conjunction of BT extract, in 1M HCl.

Percentage inhibition efficiency data are presented in Figure 1. via the corrosion rate computation. The obtained results confirmed that IE % increased as the BT extract concentration rose. The absorption of BT extract onto mild steel surfaces, which stopped active metal sites and avoided the corrosive attack by acid solution, is the basis for this increase in the number of components in BT extract. In addition, a temperature increase from 293 to 323K resulted in a substantial increase in the IE % (77.56% - 84.95%), owing to the thermal stability and inhibition performance of BT extract at high temperatures. Further increase in solution temperature to a value of 333 K led to a reduction in IE % (79.51%) which was most closely related to the deterioration of BT extract substance at high temperature. The increased ionic mobility may have influenced the protective activity of BT extract at the metal/electrolyte interface, which was blocked at elevated temperatures [20]. However, the direct link between the inhibitor efficiency and BT extract concentration was seen in the medium of 1 M HCl aggressiveness.

3.3. Kinetic and thermodynamic parameters

To measure kinetic and thermodynamic properties, mild steel corrosion in differing concentrations of BT was employed at various temperatures. The

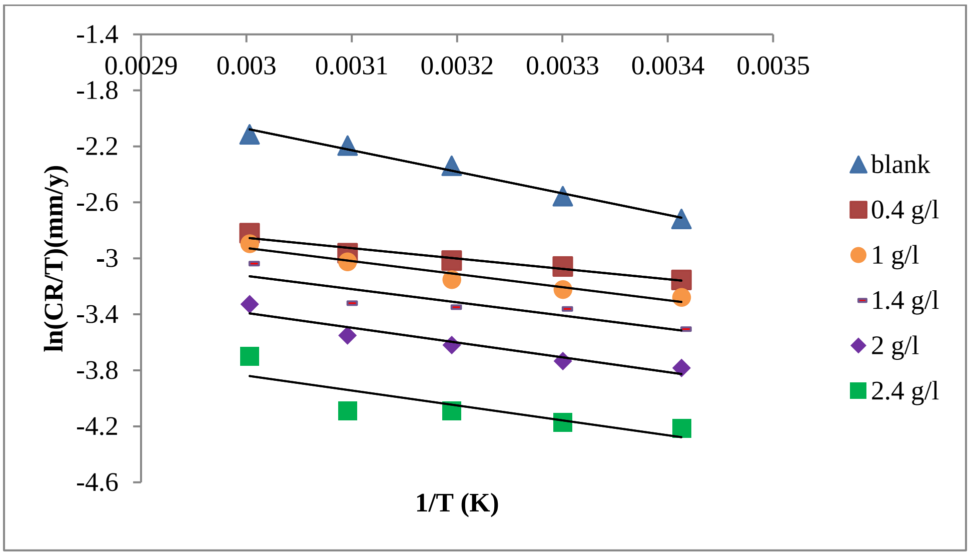

Figure 3. A graph of ln (CR/T) with 1/T with different concentrate levels of BT.

Table 2. Thermodynamic parameters at various BT concentrations.

Concentration of BT(g/l)	Ea (kJ/mol)	ΔH° (kJ/mol)	-ΔS° (J/mol.K)
Blank	15.38	12.79	21.15
0.4	8.74	6.15	5.26
1	10.35	7.76	1.06
1.4	10.45	7.85	2.42
2	11.38	8.78	1.83
2.4	11.45	8.86	5.33

Arrhenius Equation 3 [21] can be utilized to form kinetic information.

$$\ln (CR) = B - \frac{E_a}{RT} \quad (3)$$

B is the metal-dependent Arrhenius constant, whereas R is the 8.314 J/mol.k uniform gas constant. The activation energy (Ea) was computed from a slope of an ln CR against 1/T presented in Figure 2. The enthalpy (ΔH°) and entropy (ΔS°) were computed by the transition state Equation 4.

$$CR = \frac{RT}{Nh} \exp\left(\frac{\Delta S^o}{RT}\right) \exp\left(\frac{-\Delta H^o}{RT}\right) \quad (4)$$

N denotes Avogadro's number, and h refers to Planck's variable. After plotting ln (CR/T) versus 1/T, the magnitude of ΔH° and ΔS° were determined from a straight line with a slope and intercept as shown in Figure 4. Then, the obtained results are demonstrated by Table 2.

In the presence of BT extract, BT molecules absorbed on a metal surface [22] may require relatively low activation energy values. BT extract may also have antioxidant properties [22]. Furthermore, the decrease in Ea values observed in treated specimens was attributed to the coordination compound generated between metal and BT extract molecules. This action effectively ensured that the thick blocking layer was generated by BT extraction. A thick film hampered steel dissolution because of the hydrocarbon chain orientation to the acid solution [23,24].

3.4. Adsorption isotherm and Gibbs energy

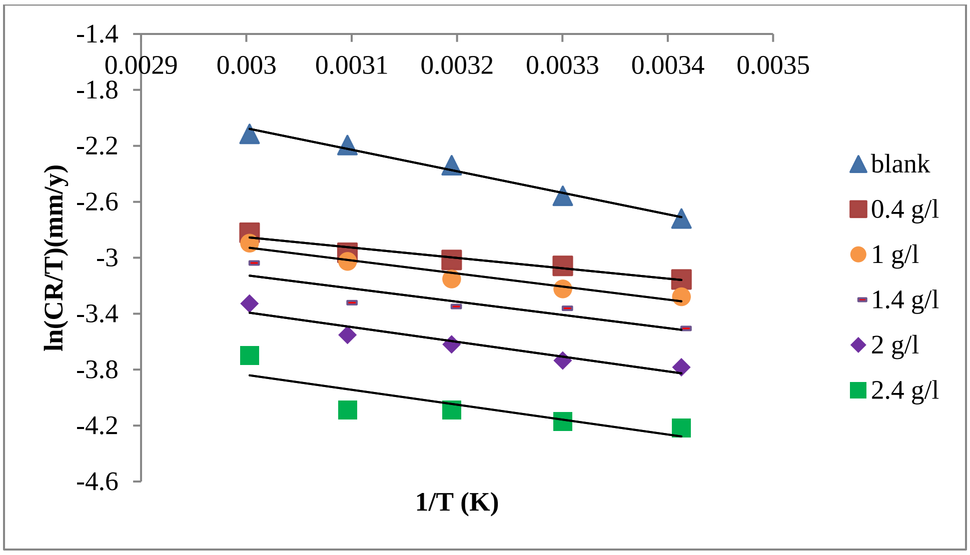

Figure 4. Isotherms mode of black tea extract at various temperature.

Table 3. The adsorption features of BT extract on a mild steel surface at multiple temperatures.

Temperature (K)	K_{ad} $(g/l)^{-1}$	ΔG_{ad} (kJ/mole)	ΔH_{ad} (kJ/mole)	ΔS_{ad} (J/mole. K)
293	0.929	-9.61	-14.014	0.811
303	1.095	-10.38		
313	1.6736	-11.79		
323	1.848	-12.43		
333	1.728	-12.64		

For the corrosion inhibition tendency of organic molecules, meeting inhibitor particles and metal surfaces through the adsorption action can be imperative. The adsorbed film created at a specific temperature, dependent on the concentration of BT extract, was computed using Surface Coverage (ϴ) Equation 5.

$$\Theta = IE / 100 \quad (5)$$

The surface coverage obtained was used to classify the fitted adsorption isotherm type BT extract's inhibitory properties may be explained by the adsorption of BT extract onto mild steel surfaces, forming a passive film. The surface coverage ϴ increased as the extract concentration in all tested temperatures (293 to 333 K) rose. This indicates that BT extracts adsorb onto the surfaces of metal substrates. According to the plot C_{inh}/Θ vs C_{inh} at different temperatures, as shown in Figure 4. a linear trend with slop and correlation coefficient R^2 approximately equal to one, the adsorption type was followed Langmuir adsorption isotherm as given in Equation 6 [26].

$$\frac{C_{inh}}{\theta} = \frac{1}{K_{ad}} + c_{inh} \quad (6)$$

The adsorption constant is K_{ad}, while the BT concentration is C_{inh}. By intercepting the lines with the x-axis, the magnitude of K_{ad} and free standard energy ΔG are determined from Equation 7. [26].

$$K_{ad} = \frac{1}{55.5} \exp\left(\frac{\Delta G_{ad}}{RT}\right) \quad (7)$$

The modified Gibbs–Helmholtz Equations 8. [27] applied to compute the thermodynamic properties of adsorption, including enthalpy ΔH_{ad} (kJ/ mol) and entropy ΔS_{ad} (kJ/mol).

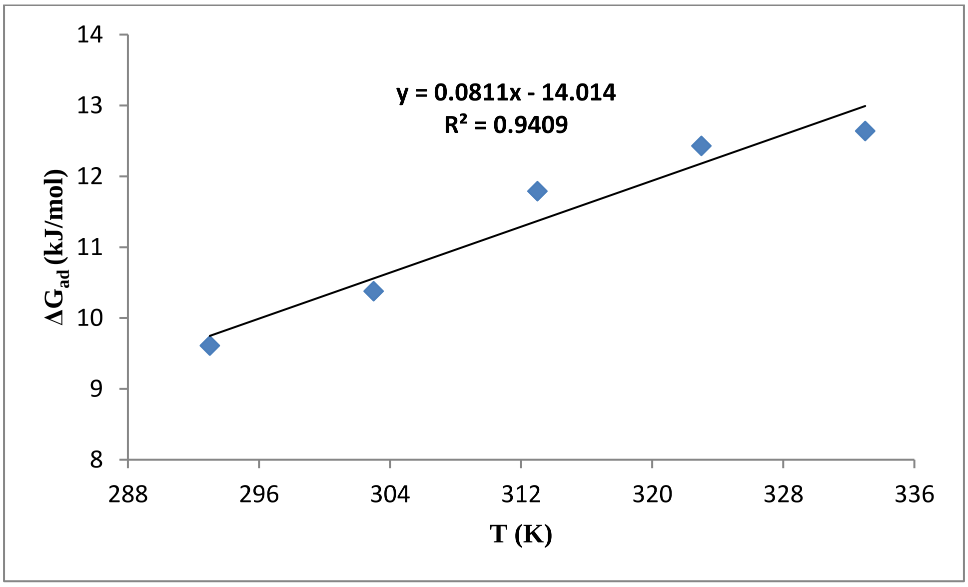

Figure 5. The variation of ΔG (kJ/mol) as a function of temperature (K) for mild steel in 1 M HCl.

$$\Delta G_{ad} = \Delta H_{ad} - T.\Delta S_{ad} \quad (8)$$

The parameter that had been obtained was listed in Table (3). It was deduced that increasing temperature from (293 to 333 K) led to k_{ad} increase from 0.929 to 1.728 $(g/l)^{-1}$. The term referred to the increase in interactions between BT molecules and a mild steel surface [28].

When the ΔG_{ad} was about -20 kJ/mol or even less, it implied a physisorption interaction, demonstrating the moves to the surface of the metal or charge sharing. The data decreased toward more negative values (9.61 to 12.64) kJ/mol as the temperature rose from 293 to 333 K. A protective passive layer in the acid medium was created when BT species adsorbed spontaneously on mild steel surfaces [30]. A linear trend with a coefficient of correlation of 0.9409 as shown by Figure 5, indicated the plot of ΔG_{ad} against the value of temperature. Also, the slope and intercept of the linear relationship depicted in Table 3. have been applied to compute the standard (ΔH_{ad}) and (ΔS_{ad}). In the interaction between mild steel surface and BT extract molecules [28,29], the negative signal of (ΔH_{ad}) suggested an exothermic adsorption procedure. Thus, mild steel dissolution was triggered by ionic species migration to the barrier layer. The study also assisted mild steel surface hydrophilization with a higher temperature and BT concentration [30,31]. The adsorption process of BT extracts on metal surfaces has increased the disorder which can be demonstrated by the obtained positive magnitude of the entropy (ΔS +0.0811). Concerning research, both chemisorption and physisorption are essential for the green inhibitor ability of BT extract on mild steel in 1 M HCl.

4. CONCLUSIONS

- BT extract showed a significant inhibitory effect in the acid solution when the CR of mild steel decreased and IE % improved over all investigations. When the temperature was increased from 293 to 323 K, the IE % rose from 77.56% to 84.95%, with the highest extraction of 2.4 g/l. As the temperature was elevated to 333 K, the IE% decreased to 79.51%, suggesting that the barrier layer deteriorated. However, as the temperature was higher than 333 K, the corrosion rate began to increase; consequently, demonstrating that the barrier layer had deteriorated slightly due to exposure to high temperatures.
- At ambient temperature and various BT concentrations ranging from (0.4 - 2.4 g/l), the results confirmed an enhancement in the IE % value from 35.33 % to 77.51%.
- The adsorption of BT extract on mild steel follows the Langmuir adsorption isotherm.
- A spontaneous adsorbed of the BT particles on the metal surface occurred according to the negative magnitude of ΔG_{ad}.
- Due to the favorable kinetics and thermodynamic characteristics, the action of BT molecules implied chemisorption and physisorption processes on mild steel surfaces.

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RESEARCH ARTICLE

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Impurity and Vacancy analysis in Zig-Zag (8,0) carbon nanotubes

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ABSTRACT

Nanoscience and nanotechnology have generated billions of dollars annually, generating jobs and new products. This is an area that involves the study and manipulation of nanoscale materials (nanomaterials, on the order of 10^{-9} m). One class of nanomaterials that has aroused significant interest in the scientific community are those carbon compounds (examples include graphene, carbon nanotubes and fullerenes), especially due to their potential applications in industry. In the present work, we carried out a study on defects (absence of carbon atoms) and Ni doping in the electronic properties of a zigzag carbon nanotube containing 32 carbon atoms. Our results indicated semiconductor behavior when two vacancies are present in the structure and also an increase in the energy level of the conduction band, valence band and Fermi level when the systems are doped with Ni. Finally, for systems doped with Ni, there was a greater probability of charge exchange occurring between the 2p orbitals of carbon and the 2p orbitals of carbon to the 3d orbitals of Nickel.

1. INTRODUCTION

Nanotechnology is an area that has always been shown to be very present in our lives, even without us realizing its presence. In recent decades, it has experienced rapid growth, impacting fields such as science, technology, and healthcare [1]. It is a technology that seeks to understand a system on a nanoscale, with precision from atom to atom, to create structures with a distinctive organization capable of exhibiting behaviors and properties different from commonly known materials [2]. There are various fields that benefit from the applications of nanotechnology products, including electronics, cosmetics, agriculture, medicine, among others. One of the several products derived from nanotechnology that is widely used are carbon nanotubes (CNTs). Some examples of applications include: Catalysis, photocatalysis and photoelectrocatalysis. For example, CNTs combined with titanium dioxide (TiO_2) have been used in photocatalysis to generate hydrogen from water [3]. According to Herbst, Macêdo, and Rocco, CNTs are formed from hexagonal arrangements of carbon that give rise to small cylinders [4]. Carbon nanotubes can be classified based on their structure and the arrangement of carbon atoms along the nanotube. Considering the structure, carbon nanotubes can be divided into single-walled carbon nanotubes (SWCNTs) and multi-walled carbon nanotubes (MWCNTs) (Figure 1). Single-walled carbon nanotubes consist of a single sheet of graphene rolled into a cylindrical shape. When nanotubes include other nanotubes, they are referred to as multi-walled carbon nanotubes.

When analyzing the arrangement of atoms, carbon nanotubes can be classified into three categories: armchair, zigzag, and chiral. We can characterize the structure of an SWCNT as a pair of indices (n, m) that describe the chiral vector and directly have an effect on electrical properties of

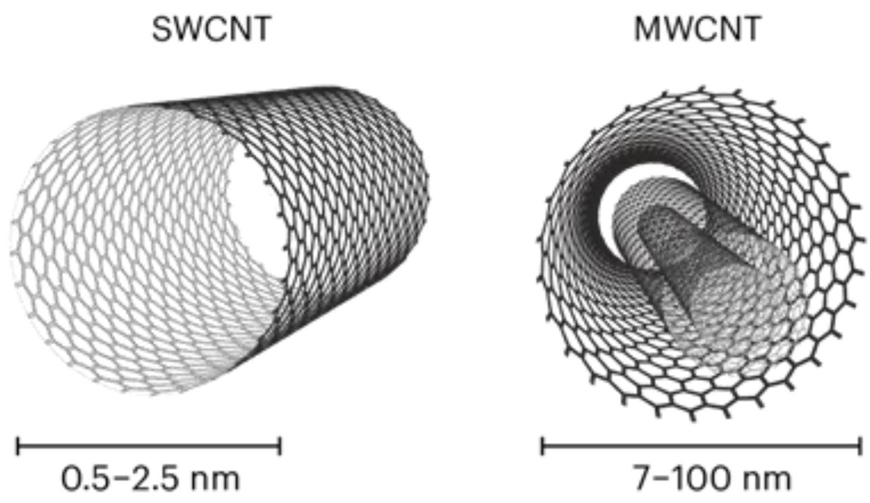

Figure 1. Single-walled nanotubes (left) and multi-walled nanotubes (right). Source: [5].

nanotubes. The number of unit vectors in the honeycomb crystal lattice of graphene along two directions is determined by the integers n and m. As a common opinion, when m = 0, the nanotubes are named zigzag nanotubes; when n = m, the nanotubes are named armchair nanotubes, and other state are called chiral [6] (Figure 2).

The properties exhibited by carbon nanotubes vary depending on the category in which they are classified: carbon nanotubes can “grow” in a different pattern. Although each tube has the same ingredient (carbon atoms arranged in a hexagonal lattice), the level of conductivity varies with chirality (the angle at which this carbon sheet is oriented relative to the tube axis). It ranges from metallic for “armchair” tubes to semiconductor in the case of “zigzag” or “chiral” tubes [5].

During the manufacturing process of carbon nanotubes, defects may occur, such as the absence of atoms. Such defects may interfere with their chemical and physical properties. In general, defects can modify the properties of carbon nanotubes depending on the method used to generate them, their concentration, and the type of nanotubes. In some cases, defects can help increase the adhesion of carbon nanotubes to a

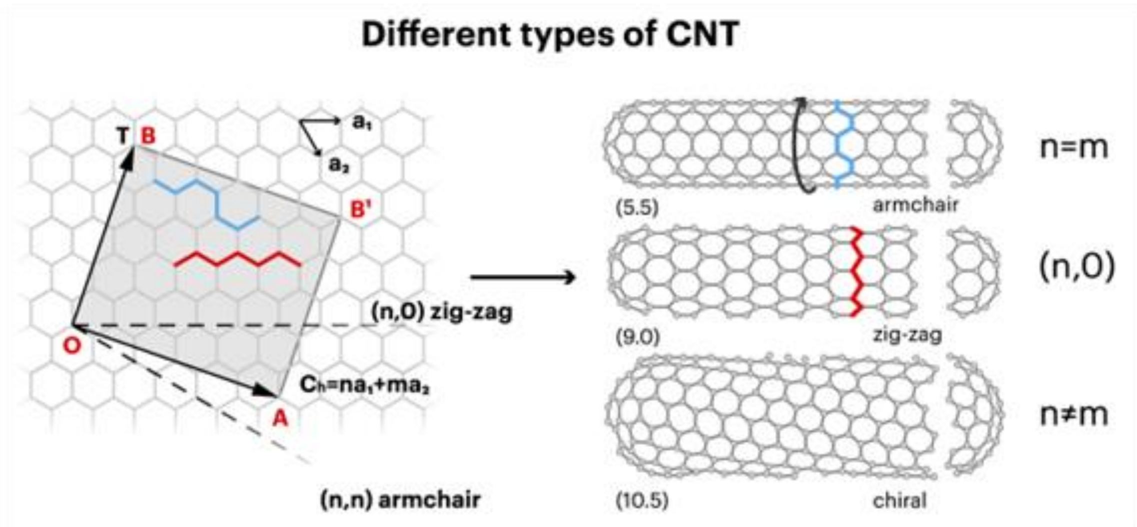

Figure 2. Different types of carbon nanotubes in terms of atom arrangement. Source: [5].

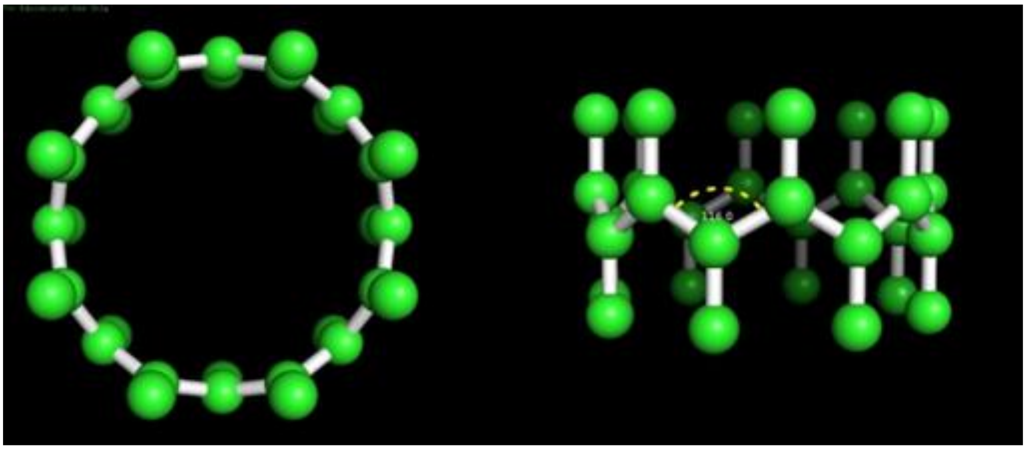

Figure 3. Defect free carbon nanotube.

polymer matrix, when mixing them to create a composite material. This could be beneficial to both the mechanical and electrical behavior of polymer nanocomposites that use CNT as fillers. Also, defects could improve the properties of carbon nanotube bundles by helping create defect-mediated covalent bonds between SWCNTs in bundles or between shells of MWCNTs. In carbon nanotubes, defects can be generated, for example, by irradiation or by chemical treatment [7].

As this is a quite common situation, the aim of this work is to conduct a study on defects in carbon nanotubes and additionally the effect of Nickel doping and how they can affect their properties.

2. METHODOLOGY

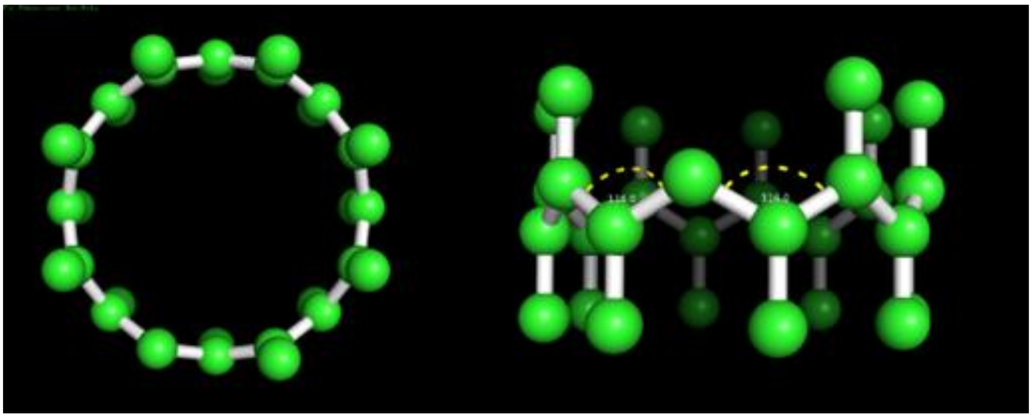

Figure 4. Carbon nanotube with one carbon vacancy.

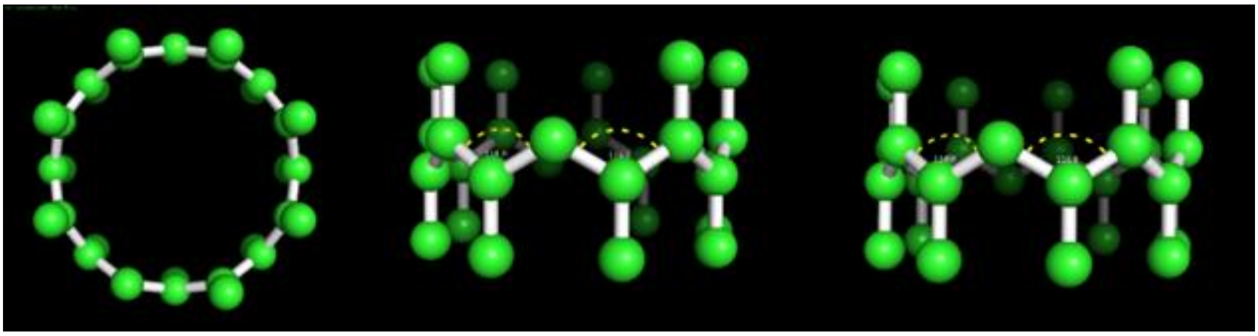

Figure 5. Carbon nanotube with two carbon vacancies. The middle figure shows one side where a carbon has been removed, and the figure on the right indicates the immediately opposite side.

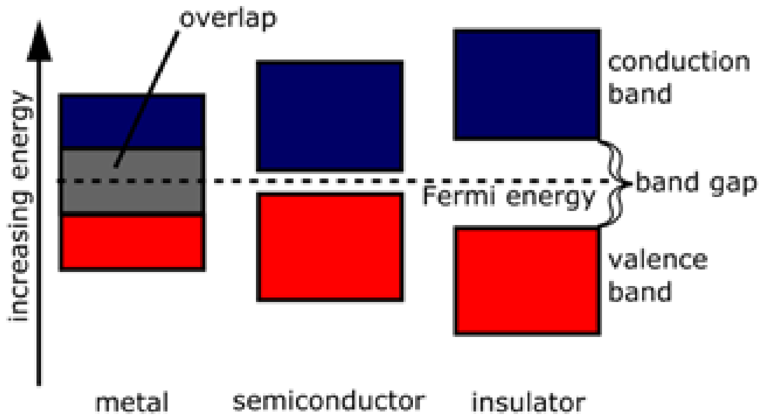

Figure 6. Illustration of the band gap. Source: Adapted from the reference [13].

In this work, a (8,0) zigzag-type carbon nanotube (CNT) composed of 32 carbon atoms was used to analyze the effects of carbon atom vacancies and Ni impurity on the electronic structure. The distance between carbon atoms (C-C) was between 141 Å and 1.42 Å, and the angle between three carbon atoms was 116º (Figure 3). Figures 3, 4 and 5 were generated by the pymol program [8]. The structure of the CNT, together with the input files for the Siesta program [9] used in this work, was obtained from Castillo's work [7]. The method employed in this work and implemented in Siesta was Density Functional Theory (DFT), and the exchange-correlation functional used was of the local density approximation (LDA) type with the CA parameterization. The carbon atom pseudopotential required for the calculations was obtained from the reference [10]. A thermodynamic correction was applied for a temperature of 300 K, with a kinetic energy cutoff for plane waves set at 300 Ry, and the following symmetry points were used to analyze the solid-state energy bands: G (0, 0, 0) and X (0, 0, 1). These points are in the unit cell constant with a value of 4.257 Å, considering a cubic unit cell with parameters a = b = c = 4.257 Å and α = β = γ = 90º. A relaxation of the structure coordinates was allowed through a geometry optimization using conjugate gradients with 200 steps and a force minimization criterion between atoms of 0.04 eV/Ang.

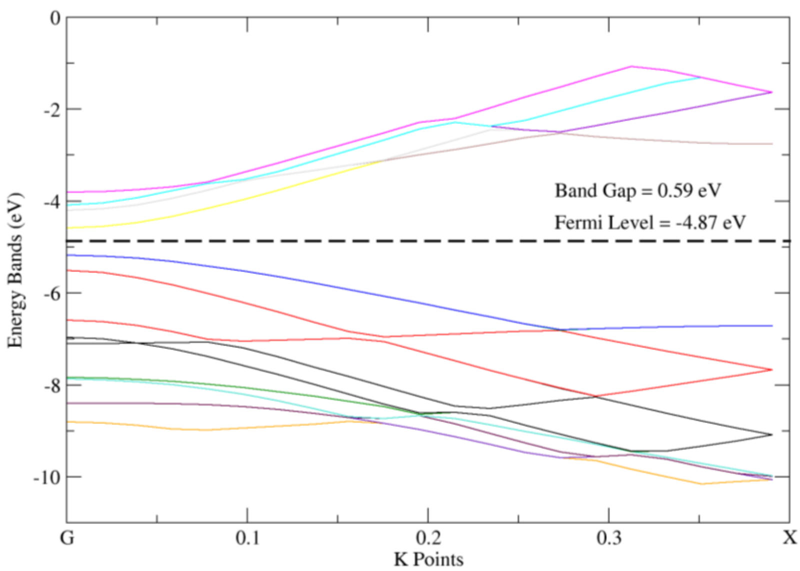

Figure 7. Energy band diagram of a nanotube without carbon vacancies. Source: Adapted from the reference [7].

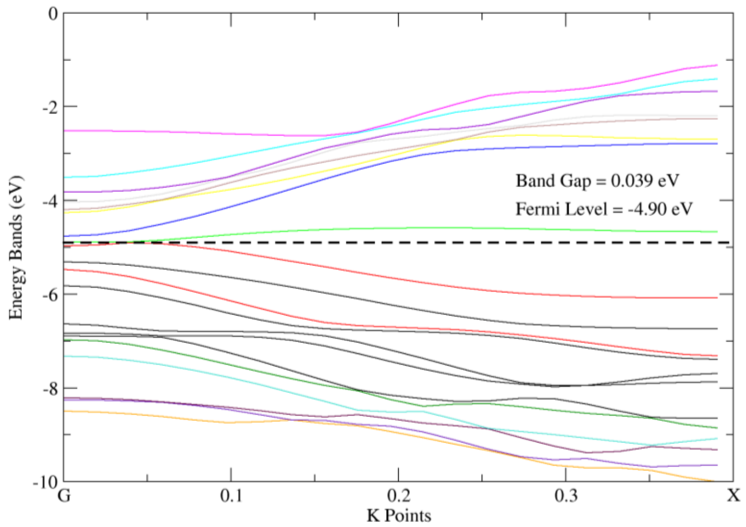

Figure 8. Energy band diagram of a nanotube with the vacancy of one carbon. Source: Adapted from the reference [7].

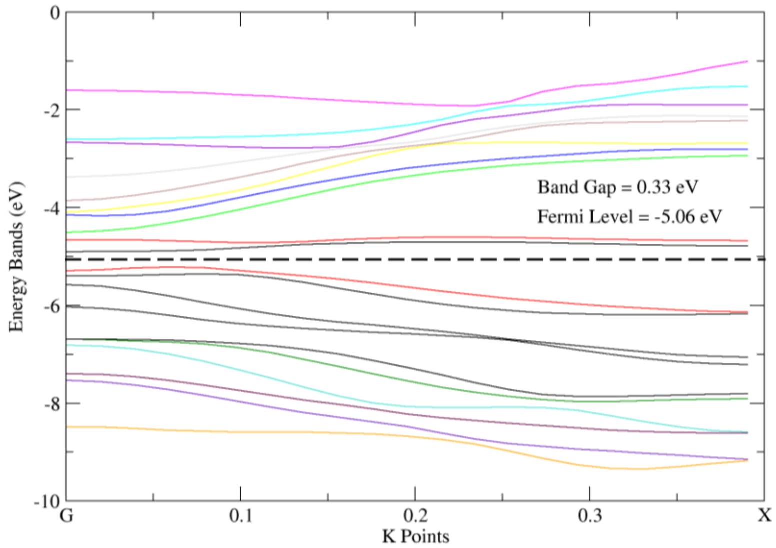

Figure 9. Energy band diagram of a nanotube with the vacancy of two carbons. Source: present work.

We use a supplementary program in Mathematica [11] and the Siesta utility programs to format the output data from the Siesta program into a format that can be recognized by GRACE [12]. With the data organized, we constructed the energy bands and density of states for each nanotube.

3. RESULTS AND DISCUSSION

After the calculations were performed, it was possible to calculate the band gap value of each nanotube. The "band gap" (E_g) consists of the separation between the valence band and the conduction band of the solid (Figure 6).

Insulating materials have $E_g > 4$ eV, semiconducting materials have $E_g < 4$ eV, and metallic materials have $E_g \approx 0$.

In Figures 7 (defect-free), 8 (one carbon vacancy), and 9 (two carbon vacancies), we present the energy band graphs of the CNT as a function of the k-points and also the Fermi energy and the value of E_g.

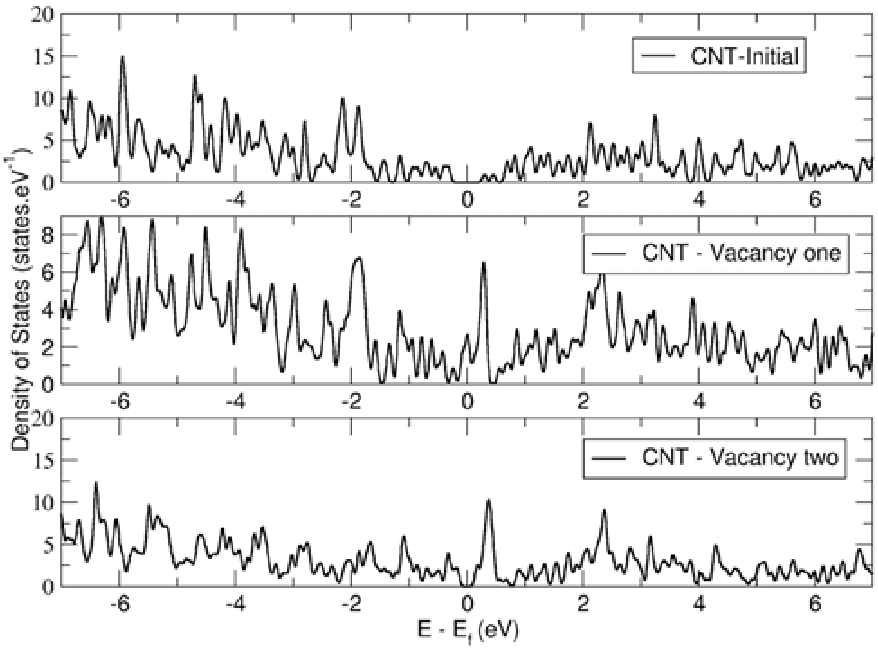

Figure 10. Density of states for three cases studied this work. Source: present work.

Removing a carbon atom causes an overlap of the valence and conduction bands, causing it to transition from a semiconductor state (E_g = 0.5898 eV) to a metallic one (E_g = 0.039 eV) [7]. When two carbon atoms are removed, the nanotube reverts back to exhibiting semiconductor properties (E_g = 0.326 eV). We attempted to replicate these defects in different positions/another carbon atoms, the results didn't change. These results are in agreement with those obtained by Orellana and Fuentealba [14] who carried out studies with (10,0) and (14,0) zigzag CNT using computational methods similar to those used in the present work.

Figure 10 displays the density of states (DOS) for the three cases mentioned above. The Fermi level is located at the origin of the abscissa axis and one can clearly see an absence of separation of density of states at the Fermi level, indicating a metallic character for the graph with one vacancy. With two vacancies, a slight separation of the density of states at the Fermi level is observed, indicating semiconductor behavior like the primitive CNT in agreement with the literature.

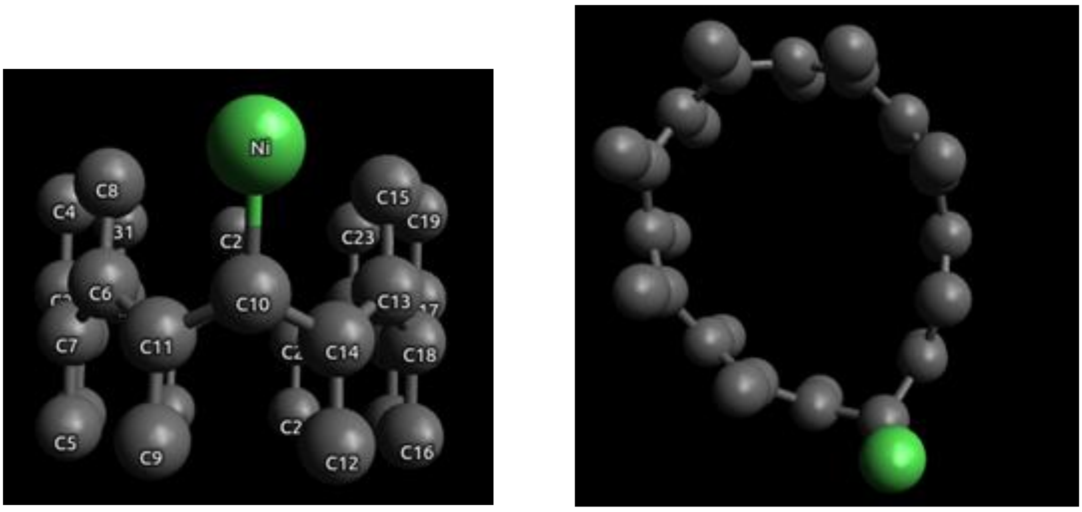

Figure 11. CNT doped with Ni. Source: present work.

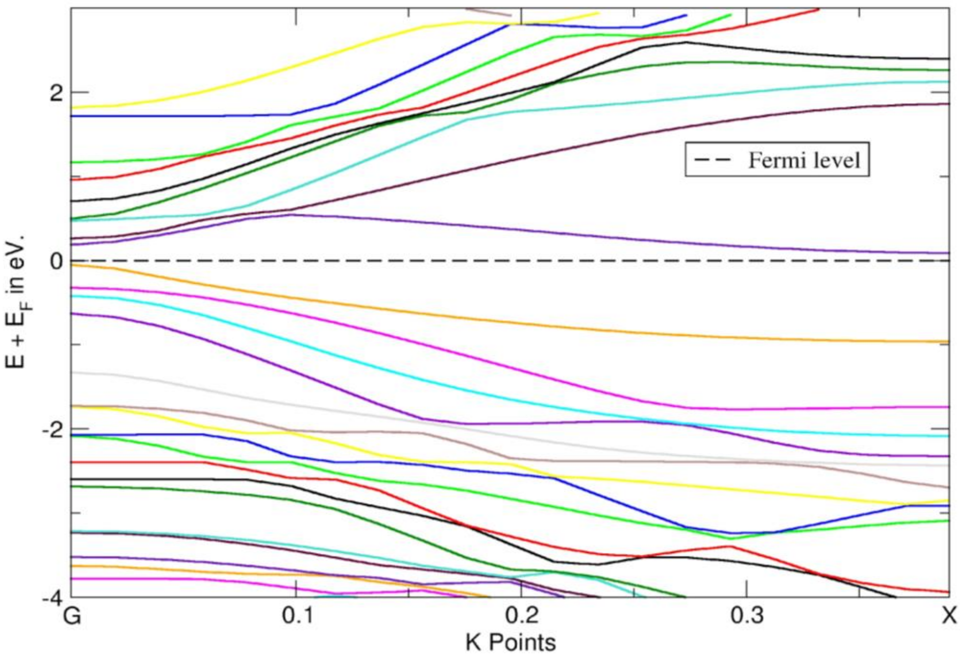

Figure 12. Energy band diagram of a nanotube doped with one Ni. Source: present work.

The inclusion of impurities composed of transition elements from the periodic table in CNT has indicated important applications in energy storage. For example, Yang and collaborators [15] carried out doping (by replacing a carbon atom) of an armchair CNT with chiral indices (6,6) with the following transition metals Sc, Ti, V, Cr, Mn, Fe, Co, Ni, Cu and Zn and investigated quantum capacitance and electronic structure. The results indicated that doping with transition elements improves the quantum capacitance of carbon nanotube electrodes. The highest quantum capacitance was obtained with Ni doping [15]. Azevedo and collaborators [16] carried out the doping (by adding an impurity inside the carbon nanotube) of ziz-zag type CNT containing 64

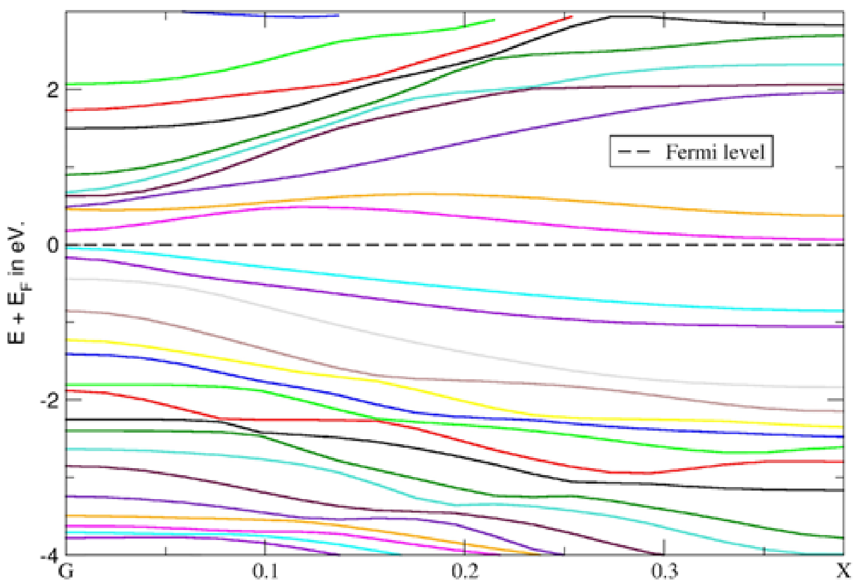

Figure 13. Energy band diagram of a nanotube with one vacancia doped with Ni. Source: present work.

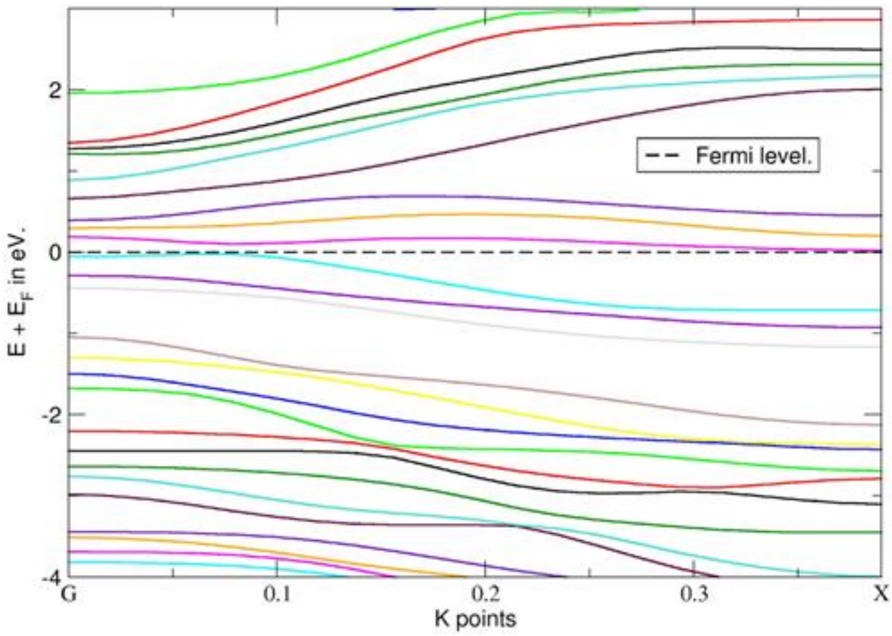

Figure 14. Energy band diagram of a nanotube with two vacancies doped with Ni. Source: present work.

carbon atoms with the Fe, Ni and Mn transition metals. They investigated the diameter's effect on stability and electronic properties. Some of the results indicated that the magnetization depends on the radius of curvature and increases with Mn impurities and decreases with Fe and Ni impurities. With the aim of contributing to the understanding of the behavior of impurities of transition elements in CNT in the present work we also investigated the behavior of the three cases discussed previously after doping with Ni atoms. We randomly replace a carbon atom by a Ni atom.

Figure 11 displays the molecular geometry after Ni inclusion and structure optimization. Regarding

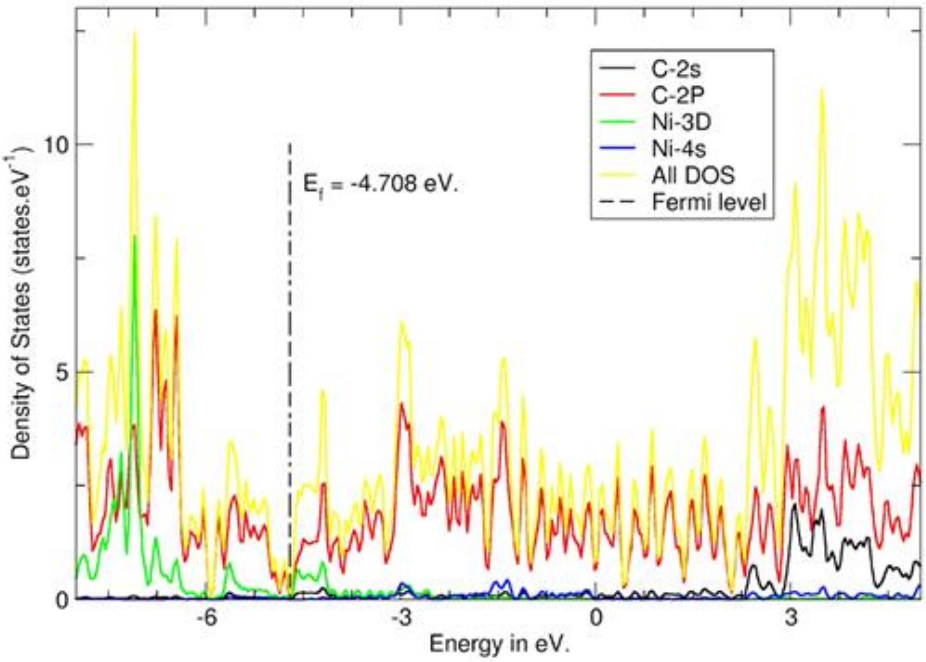

Figure 15. Partial and total density of states of the initial Structure doped with one Ni impurity (C31Ni).

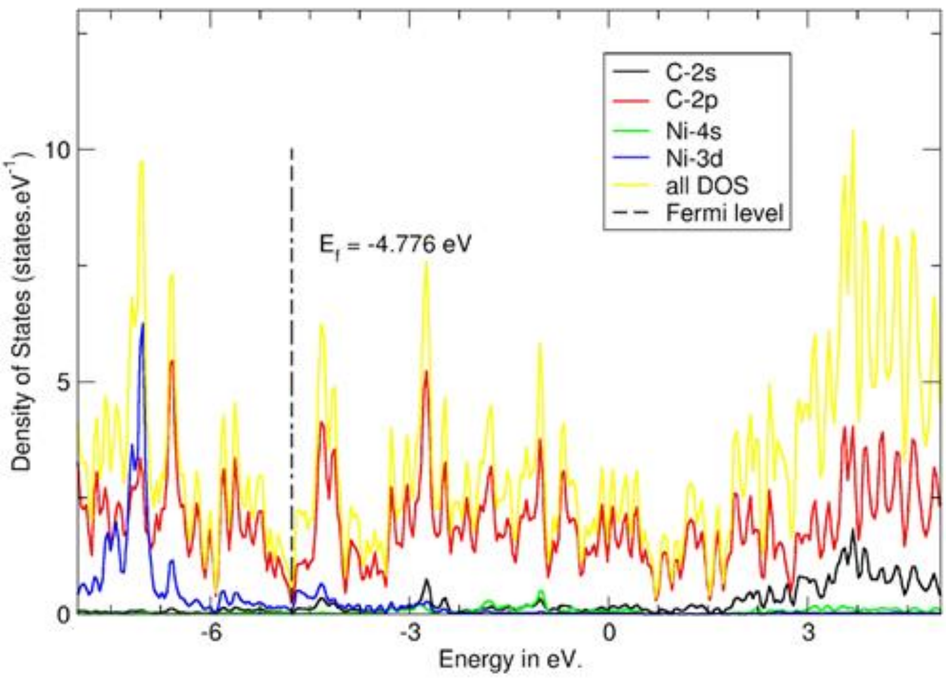

Figure 16. Partial and total density of states of the initial Structure doped with one Ni impurity and with one vacancy (C30Ni).

the bond length, the most abrupt changes occurred in the bonds between C10 - Ni (from 142 Å to 1.82 Å), C11 - C10 and C14 - C10 (from 141 Å to 1.49 Å). For the angular dimension, the most abrupt

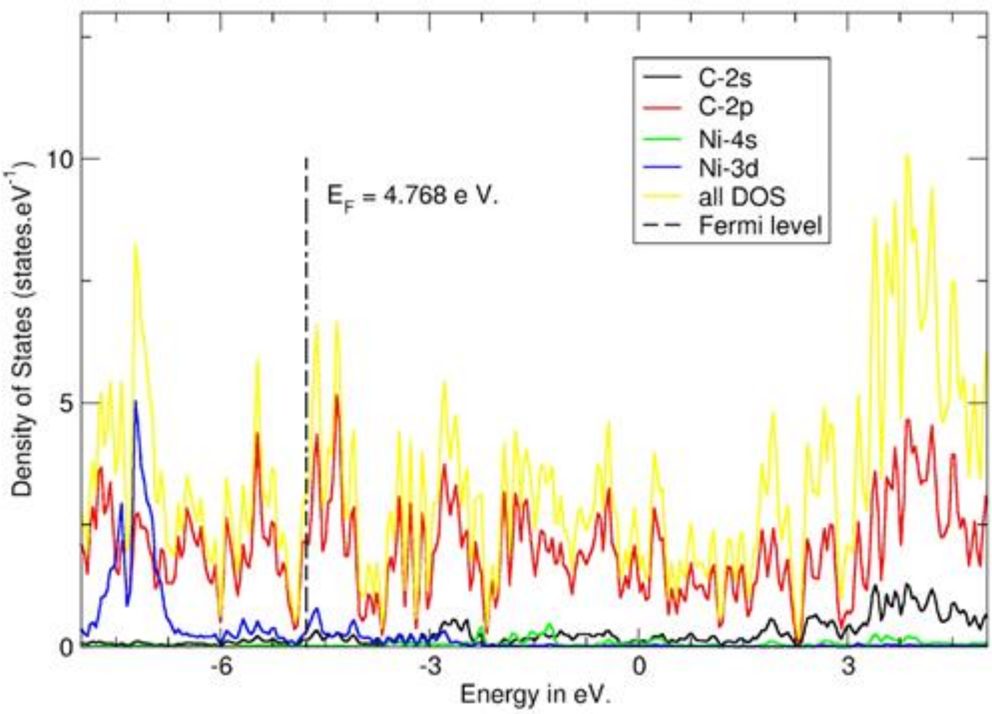

Figure 17. Partial and total density of states of the initial Structure doped with one Ni impurity and with two vacancy (C29Ni).

Table 1. Properties of nanotubes calculated in the present work.

Nanotube	valence band energy (in eV)	conduction band energy (in eV)	Fermi level (in eV)	Band gap (in eV)	behavior
C32	-5.18	-4.59	-4.87	0.59	semicondutor
C31	-4.92	-4.89	-4.90	0.04	metallic
C30	-5.23	-4.90	-5.06	0.33	semicondutor
C31Ni	-4.76	-4.62	-4.71	0.14	semicondutor
C30Ni	-4.82	-4.71	-4.78	0.11	semicondutor
C29Ni	-4.89	-4.58	-4.74	0.15	semicondutor

changes occurred for the angles between C6-C11-C10 and C10-C14-C13 (from 116º to 127º).

Figures 12, 13 and 14 show the energy bands with the Fermi level centred at the origin. The Fermi level was - 4.71 eV, - 4.78 eV and 4.74 eV and the band gaps were 0.14 eV, 0.11 eV and 0.15 eV for C31Ni (without vacancy), C30Ni (one vacancy), and C29Ni (two vacancy), respectively. The inclusion of Ni led to semiconducting behaviour in all three cases.

Figures 15, 16 and 17 show the density of states for the three cases C31Ni, C30Ni and C29Ni respectively:

For the three cases, we can observe, analyzing the densities of states, a greater probability of charge exchange occurring, between the valence and conduction bands, from the 2p orbitals to the 2p orbitals of carbon and from the 2p orbitals of carbon to the 3d orbitals of Nickel. In the present work, we do not consider the effect of spin polarization in our calculations.

Table 1 displays all the values of the properties calculated in the present work. We rounded to two decimal places.

It can be seen in table 1 that the presence of Ni increases the energy levels of the valence and conduction bands as well as the Fermi level, therefore explaining the change from metallic behavior (C31) to semiconductor (C30Ni) after doping with Ni.

4. CONCLUSIONS

In the present work, we present a study of the effect of carbon vacancies and Ni impurities on the electronic properties of zigzag-type CNT with chiral indices (8.0) and with 32 carbon atoms. Analyzes of energy bands and density of states were carried out in the absence of one and two carbon atoms and also analysis of these systems doped with Ni. Analysis of the results led to the following conclusions:

1 – Regardless of the position from which a carbon atom is removed, CNT behaves like a metallic material.

2 – Regardless of the position from which two carbon atoms are removed, the CNT once again behaves like a semiconductor material.

3 - For systems doped with Ni, it was found that the greatest probability of charge exchange occurring is from the 2p orbitals to the 2p orbitals of carbon and from the 2p orbitals of carbon to the 3d orbitals of Nickel.

4 – The presence of Ni increases the energy levels of the valence and conduction bands, as well as the Fermi level, therefore explaining the change from the metallic behavior of C31 CNT to the semiconductor behavior of 30Ni CNT after doping with Ni.

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