CHEMICAL SYNTHESIS OF MAGNESIUM OXIDE NANOPARTICLES

PROJECT REPORT

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CERTIFICATE

This is to certify that the project report entitled **"CHEMICAL SYNTHESIS OF MAGNESIUM OXIDE NANOPARTICLES"** is an authentic work done by ANNA OLIVIA, MELISSA E REYNOLDS and ANNS MARIA T.M, St. Teresa's College (Autonomous), Ernakulam, under my supervision at Department of Physics, St Teresa's College (Autonomous), Ernakulam, for the partial requirements for the award of Degree of Bachelor of Science in Physics during the academic year 2022-23. The work presented in this dissertation has not been submitted for any other degree in this or any other university.

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DECLARATION

WE, ANNA OLIVIA , ANNS MARIA T.M, MELISSA E REYNOLDS, final year B.Sc. Physics students, Department of Physics, St. Teresa's College (Autonomous) , Ernakulam, do hereby declare that the project work entitled "**CHEMICAL SYNTHESIS OF MAGNESIUM OXIDE NANOPARTICLES"**, has been originally carried out under the guidance and supervision of Smt. DR. PRIYA PARVATHI AMEENA JOSE, Assistant Professor, Department Of Physics, St. Teresa's College (Autonomous), Ernakulam, in partial fulfilment for the award of the degree of Bachelor of Physics. I further declare that this project is not partially or wholly submitted for any other purpose and the data included in the project is collected from various sources and are true to the best of my knowledge.

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CHEMICAL SYNTHESIS OF MAGNESIUM OXIDE NANOPARTICLES

ABSTRACT

Nanoscience and nanotechnology represent an expanding research area, which involves structures, devices, and systems with novel properties and functions due to the arrangement of their atoms on the 1–100 nm scale. Metal Oxide nanoparticles constitute a fascinating class of inorganic solids, which have attracted the attention of materials scientists and engineers. Their magnetic, electrical, optical, catalytic and mechanical properties make them technologically useful.

Synthesis of metal oxide nanoparticles can be done through different methods like physical, chemical and green methods. Present work focus on the synthesis of MgO nanoparticles by chemical method using $Mg(NO_3)_2$ and NaOH, a non-toxic and eco-friendly one. The NaOH acts as a reducing agent in the reaction. The particles thereby obtained were characterized by XRD analysis and calculated the average particle size.

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CHAPTER – 1

INTRODUCTION

1.1 NANOSCIENCE AND NANOTECHNOLOGY

Nano science is an emerging area of science which concerts itself with the study of materials that have very small dimensions, in the range of Nano scale. The word Nano science itself a combination of Nano, from Greek "Nanos" meaning "Dwarf", and the word "Science" meaning knowledge. The prefix Nano simply means one billionth. So, one Nanometre (nm) is 10^{-9} m. to help put this size in perspective, one-tenth of 1 nm is approximately the size of an atom.

It is not just the science of small, but the science in which materials with small dimension show new physical phenomena, collectively called quantum effect, which are size dependent and dramatically different from the properties of macro-scale materials. Hence it makes the field of science that measures and explains the changes of the properties of substances as a function of Nano size.

The usage of science and technology by the society is an indirect measure of advancement and development, and often the nature of the society is known by the technology it excels in. Therefore, the societies have evolved from agriculture based to industry based, and further from information to communications and technology based.

There has been a technology explosion in the last few years due to various new tools and techniques for the creation, characterization and manipulation of materials at the scale of nanometre. Generally speaking, Nanotechnology represents the design, characterization, production and application of structures, devices and systems by controlling shape and size with Nano specifications. The technology to create, observe and manipulate matters at the nanometre scale is probably the very field where different disciplines, such as physics, chemistry, material science, engineering, biology and medicine, combine to offer immense opportunities and challenges.

Thus, it would bring about a major revolution and influence on the way we live today. The vast global on these technologies is going to make the world more competitive in terms of both knowledge and the use of these technologies.

Even though nanometre scale is commonly indicated as 1-100 nm, but Nano science and nanotechnology often deal with objects larger than 100nm. The variability arises from the interdisciplinary nature of nanotechnology, which arises from the convergence of chemistry, physics and material sciences, engineering, molecular biology, biology and medicine. In some fields objects studied are in the 1-100 nm length scale (e.g., quantum dots), but in other fields, such as biochips, objects have dimensions in the range of hundreds of nanometres. Even though Nano science is often perceived as a science of the future, it is actually the basis for all systems in our living world.

Nanotechnology should not be viewed as a single technique that only affects specific areas. Although often referred to as the 'tiny science', nanotechnology does not simply mean very small structures and products. Nano scale features are often incorporated into bulk materials and large surfaces as the materials reduced to Nano dimension or further reduced to dimensions of atoms or molecules exhibit altogether different properties. That is to say that the principles of classical physics are no longer describing their behaviour. At these dimensions, quantum mechanics principles apply. They exhibit altogether enhanced chemical, magnetic, electric, mechanic and optic properties.

It is indeed an on-going technology revolution. Today Nano world provides scientists with a rich set of materials useful for probing the fundamental nature of matter. These materials have unique structures and tunable properties. This makes them valuable for many different real world applications. In the coming years, there would hardly be any aspect of our lives where this technology would not make an impact.

Though nanotechnology is relatively new, the existence of functional devices and structures of nanometre dimension is not new. In fact such structures have existed on earth as long as life itself. It was not clear when humans first began to take advantage of Nano-sized materials. In the 4th century AD, Roman glass makers fabricated glass containing Nano-sized metals. In 1857, Michael Faraday discovered colloidal gold and introduced these "colloidal gold" samples to the Royal Society, the suspension of gold nanoparticles in the solution was totally transparent in some lighting, but in other lighting conditions it produced differently colored solutions of "ruby, green, violet or blue". In the year 1959, on December 29th, the famous physicist Richard Feynman first pointed out

Some potential quantum benefits of miniaturization. He presented a lecture at a meeting of the American Physical Society at Caltech, entitled "There's plenty of room at the bottom" where he discussed the possibility of controlling materials at the level of atoms and molecules. This was the first mission of the possibilities of science and technology at the Nano scale. The term "nanotechnology" was defined in 1974 by Tokyo science university professor Norio Taniguchi. He used the word to refer to production technology to get the extra high accuracy and ultra-fine dimension. i.e., the preciseness and fineness of the order of 1 nm.

In 1981, Gerd Binnig and Heinrich Rohrer at IBM's Zurich lab invented the scanning tunneling microscope, allowing scientists to "see" individual atoms for the first time. Binnig and Rohrer won the Nobel Prize for this discovery in 1986. In 1985, Rice University researchers Harold Kroto, Sean O'Brien, Robert Curl, and Richard Smalley discovered the Buckminsterfullerene (Co), more commonly known as the Bucky ball, which is a molecule resembling a soccer ball in shape and composed entirely of carbon, as are graphite and diamond. The team was awarded the 1996 Nobel Prize in Chemistry for their roles in this discovery and that of the fullerene class of molecules more generally. IBM research scientists Don Eigler and Erhard Schweizer at IBM's Almaden Research Center manipulated 35 individual xenon atoms to spell out the IBM logo in 1990. This demonstration of the ability to precisely manipulate atoms ushered in the applied use of nanotechnology. Later in the year 1991 Sumio lijima was credited with discovering the carbon nanotube (CNT), although there were early observations of tubular carbon structures by others as well. CNTs, like Bucky balls, are entirely composed of carbon, but in a tubular shape. They exhibit extraordinary properties in terms of strength, electrical and thermal conductivity, among others. A method for controlled synthesis of Nano crystals (quantum dots), paving the way for applications ranging from computing to biology to high-efficiency photovoltaic and lighting was invented in 1993 by Moungi Bawendi. Within the next several years, work by other researchers such as Louis Brus and Chris Murray also contributed methods for synthesizing quantum dots. In 1999 early 2000's, Consumer products making use of nanotechnology began appearing in the marketplace providing a wide range of applications in the field of electronics, fuel cells, batteries, agriculture, food industry and medicines. Erik Winfree and Paul Rothemund in 2005 from the California Institute of Technology developed theories for DNA-based computation and "algorithmic self-assembly" in which computations are embedded in the process of Nano crystal growth. In 2007, Angela Belcher and colleagues at MIT built a lithium-ion battery with a common type of virus that is non-harmful to humans, using a low-cost and environmentally friendly process. In- between 2009-2010, Nadrian Seeman and colleagues at New York University created several DNA-like robotic Nano scale assembly devices. One is a process for creating 3D DNA structures using synthetic sequences of DNA crystals that can be programmed to self-assemble using "sticky ends' ' and placement in a set order and orientation. In the year 2010, IBM used a silicon tip measuring only a few nanometres which demonstrated a powerful patterning methodology for generating Nano scale patterns and structures as small as 15 nanometres at greatly reduced cost and complexity, opening up new prospects for fields such as electronics, optoelectronics, and medicine. Now the research and development continues which entails the application of fields of science as diverse.

1.2 WHAT DOES MAKE NANO SPECIAL?

Nano materials have the structural features in between those of atoms and the bulk materials. While most micro structured materials have similar properties to the corresponding bulk materials the properties of materials with nanometre dimensions are significantly different from those of atoms and bulk materials. This is mainly due to the nanometre size of the materials which render them: (i) large fraction of surface atoms; (ii) high surface energy; (iii) spatial confinement; (iv) reduced imperfections which do not exist in the corresponding bulk materials.

Due to their small dimensions, Nano materials have extremely large surface area to volume ratio, which makes a large to be the surface or interfacial atoms, resulting in more “surface” dependent material properties . Especially when the sizes of Nano materials are comparable to length, the entire material will be affected by the surface properties nanomaterial. This in turn may enhance or modify the properties of the bulk materials.

1.3 NANOMATERIALS AND CLASSIFICATION:

Nano materials can be metals, ceramics, polymeric materials, or composite materials. Their defining characteristic is a very small feature size in the range of 1- 100 nm.

(I) On the basis of the dimensions of the structural elements:

One-dimensional Nano materials (1D): Materials with one dimension in the nanometre scale are typically thin films or surface coatings and include the circuitry of computer chips and the antireflection and hard coatings on eyeglasses. Thin films have been developed and used for decades in various fields, such as electronics, chemistry and engineering. Thin films can be deposited by various methods and can be grown controllably to be only one atom thick, a so-called monolayer. Nanotubes, fibres, and rods are included as examples.

Two-dimensional Nano materials (2D): These Nano materials have two dimensions in the nanometre scale. It includes 2D films (coatings) having nanometre thickness with nanostructures firmly attached to a substrate, or Nano pore filters used for small particle separation and filtration. Structural elements in 1D and 2D nanomaterial can be distributed in a liquid or solid macroscopic matrix or be applied on a substrate . Asbestos fibres are an example of two dimensional nanoparticles.

Three-dimensional nanomaterial (3D): Materials that are Nano scaled in all three dimensions are considered and 3D nanomaterial. It includes powders, fibrous, multilayer and polycrystalline materials in which the 1D and 2D structural elements are in close contact with each other and form interfaces. An important type of three-dimensional nanostructure materials is a compact or bulk polycrystalline with Nano size grains, whose entire volume is filled with those Nano grains, free surface of the grains is practically absent, and there are only grain interfaces.

(II)On the basis of manufacturing approaches:

There are mainly two major approaches to get nanomaterial. One is the bottom up and the other is the top down approach.

In the **bottom up approach**, single atoms and molecules are assembled into larger nanostructures. This is a very powerful method of creating identical structures with atomic precision although to date, the man-made materials generated in this way are still much simpler than nature's complex structures. It provides components made of single molecules, which are held together by covalent bonds that are far stronger than the forces that hold macro-scale components . Furthermore, the amount of information that could be stored in devices built from the bottom up would be enormous.

The **top down approach** involves the breaking down of large pieces of material to generate the required nanostructures from them. This method is particularly suitable for making interconnected and integrated structures such as in electronic circuitry. It provides the construction of parts through methods such as in cutting, carving and moulding. Using these methods we have been able to fabricate a remarkable variety of machinery and electronic devices. However, the sizes at which we can make these devices are severely limited by our ability to cut, carve and mould.

(III) On the basis of the type of the materials:

Carbon based nanomaterial (CBN): These are defined as nanomaterial composed mostly of carbon, most commonly taking the form of hollow spheres, ellipsoidal or tubes. Spherical and ellipsoidal carbon nanomaterial is referred to as fullerenes, while cylindrical ones are called nanotubes. Carbon based nanomaterial belonging to the most intensely investigated items represent one of the most widespread material classes. These particles have many potential applications, including improved films and coatings, stronger and lighter materials and applications in electronics. There is a large number of CBNs existing which are in different states of development ranging from basic and applied research to industrial applications.

Nano-composites: It is a multiphase solid material where one of the phases has one, two or three dimensions of less than 100 nanometres, or structures having Nano-scale repeat distances between the different phases that make up the material. They are conventional materials reinforced by Nano scale particles or structures which are dispersed throughout the bulk material. The base material itself is mainly consisting of non-Nano scale matrices filled with nanomaterial. But even "Nano composites" appear where all constituents are grained in the nanometre range. Nanoparticles such as Nano-sized clays are already being added to products ranging from auto-parts to packing materials, to enhance mechanical, thermal barrier and flame retardant properties. They have found applications in battery cathodes, microelectronics, sensors etc.

Nano-ceramics: These are Nano scale particles or structures consisting of ceramic materials. Nano-ceramics include oxide and non-oxide materials. Main part of Nano-ceramic materials consists of oxide ceramics. The main non-oxide materials are nitrides and carbides. The latter are mainly appearing in hard metal composites. To achieve a concise structure, it makes sense to separate ceramic materials class roughly into oxide and non-oxide ceramics. One of the most prominent carbide ceramic nanoparticles is tungsten carbide, a chemical compound of tungsten and carbon.

Nanostructured metal and alloys: Nanostructured metal and alloys are nanoparticles, nanoparticle powder and Nano crystalline materials consisting of either a single metal or of alloys of two or more metals. They are a material class compressing a multitude of Nano scale particles and powders as well as Nano crystalline solids and nanostructures surfaces. Metal nanomaterial includes quantum dots, Nano gold, Nano silver and metal oxides, such as titanium dioxide etc. A quantum dot is a closely packed semiconductor crystal composed of hundreds or thousands of atoms, and whose size is on the order of a few nanometres to a few hundred nanometres. Changing the size of quantum dots changes their optical properties. Metallic nanomaterials have attracted particular interest due to their versatility of application in areas as diverse as catalysis, medicine and opto-electronics. More recently, silver nanoparticles were important in the photographic process and they are now finding increasing use due to their antimicrobial properties.

The desire to fabricate materials with well-defined, controllable properties and structures, on the nanometre scale, coupled with the flexibility afforded by intermetallic materials, has generated interest in bimetallic and multimetallic Nano alloys. There are a large number of combinations of metallic elements and a wide range of elemental compositions which are possibilities for Nano alloys. One of the major reasons for interest in Nano alloys is because their chemical and physical properties can be tuned by varying the composition and atomic ordering, as well as the size and shape of the particles.

1.4 APPLICATIONS:

Nano materials have a wide range of applications in the field of electronics, fuel cells, batteries, agriculture, food industry, and medicines, etc... It is evident that Nano materials split their conventional counterparts because of their superior chemical, physical, and mechanical properties and of their exceptional formability.

Transportation: Nanotechnology will enhance aerospace application and space flight as new materials will allow space shuttles to become lighter and tougher. Improved catalysts could reduce or eliminate the emission of pollutants from engines. Cerium oxide nanoparticles are used in diesel fuel to greatly increase fuel efficiency. Nanoparticles of inorganic clays and polymers will replace carbon black tires and therefore we will have environmentally friendly, wear resistant tires.

Energy storage: MgO can be used as anode materials in lithium-ion batteries, which can improve battery performance and stability.

Electronics: Improving display screens on electronic devices. This involves reducing power consumption while decreasing the weight and thickness of the screens. This can be achieved by using carbon nanotubes. Researchers are developing a type of memory chip with a projected density of one terabyte of memory per square inch or greater. Integrated Nano sensors are used for collecting, processing and communicating massive amounts of data with minimal size, weight, and power consumption.

Food: Nanotechnology is having an implement on several aspects of food science, from now food is grown to how it is packaged. Companies are developing Nano materials that will make a difference not only in the taste of food, but also in food safety, and the health benefits that food delivers.

Optics: Nanotechnology offers scratch resistant surface coatings based on Nano composites. Nano optics could allow for an increase in precession of pupil repair and other types of cases of eye surgery. Paints: Incorporating nanoparticles in paints could improve their performance. Thinner paint coatings, used for example on aircrafts, would reduce their weight. Applications might be in paints that change colour in response to change in temperature or Chemical environment or points that have reduced IR absorptivity and so reduce heat loss.

Biomedical applications: MgO nanoparticles have antimicrobial and anticancer properties and can be used in drug delivery systems, medical imaging, and tissue engineering.

Elimination of Pollutants: Nano materials possess extremely large grain boundaries relative to their grain size. Hence, they are very active in terms of their chemical, physical, and mechanical properties. Due to their enhanced chemical activity, Nano materials can be used as catalysts to react with toxic gases such as carbon monoxide and nitrogen oxide in automobile catalytic converters and power generation equipment to prevent environmental pollution arising from burning gasoline and coal.

Catalysis: Higher surface area available with the nanomaterial counterparts, Nano- catalysts tend to have exceptional surface activity. For example, reaction rate at Nano- aluminium can go so high, that it is utilized as a solid-fuel in rocket propulsion, whereas the bulk aluminium is widely used in utensils. Nano-aluminium becomes highly reactive and supplies the required thrust to send off payloads in space. Similarly, catalysts assisting or retarding the reaction rates are dependent on the surface activity, and can very well be utilized in manipulating the rate-controlling step.

1.5 METAL AND METAL OXIDE NANOPARTICLES

The existence of metallic nanoparticles in solution was first recognized by Faraday in 1857 and a quantitative explanation of their colour was given by Mie in 1908.The main characteristics of metal nanoparticles are large surface-area-to-volume ratio as compared to the bulk equivalents; large surface energies; the transition between molecular and metallic states; providing specific electronic structure (local density of states LDOS); Plasmon excitation; quantum confinement; short range ordering etc.

In recent years, researchers in the field of nanotechnology are finding that metal nanoparticles have all kinds of previously unexpected benefits in both the conventional technology and experimental medical industries. Nanoparticles research is gaining increasing interest due to their unique properties, such as increased electrical conductivity, toughness and ductility, increased hardness and strength of metals and alloys, luminescent efficiency of semiconductors, and formability of ceramics.

Many types of nanoparticles are being used for different applications, such as metallic, non-metallic and magnetic oxides. Metallic nanoparticles are of great interest due to their excellent physical and chemical properties, such as high surface-to-volume ratio and high heat transfer (thermal conductivity). Metallic nanoparticles have fascinated scientists for over a century and are now heavily utilized in biomedical sciences and engineering. Metal oxides also play a very important role in many areas of chemistry, physics and materials science. The metallic elements are able to form a large diversity of oxide compounds. In technological applications, oxides are used in the fabrication of microelectronic circuits, sensors, and piezoelectric devices, and fuel cells, coatings of surfaces against corrosion and as catalysts. In the emerging field of nanotechnology, a goal is to make nanostructures or Nano arrays with special properties with respect to those of bulk or single particle species. Oxide nanoparticles can exhibit unique physical and chemical properties due to their limited size and a high density of corner or edge surface sites. Recent advances in the design and preparation of metal and metal oxide nanoparticles have proved that a numerous variety of nanoparticles can nowadays be synthesized through different preparation routes. Syntheses of metal and metal oxide nanoparticles are important because of their novel electrical, optical, magnetic and chemical properties.

In this work we are synthesizing one of the metal oxides - Magnesium Oxide. Nanoparticles of Magnesium oxide constitute some of the most versatile and useful metal nanoparticles currently in production. They are of great interest due to its non-toxicity and environmental friendliness.

The objectives of this work are preparation of magnesium oxide nanoparticles by simple chemical methods and determination of Particle size and crystal structure by XRD technique.

CHAPTER 2

MAGNESIUM OXIDE NANOPARTICLES

2.1 BASIC PROPERTIES OF MgO

Magnesium oxide (MgO) is a chemical compound consisting of magnesium and oxygen. It is a white, odourless, crystalline solid. MgO is an electrical insulator and does not conduct electricity. It is a basic oxide and can neutralize acids to form salts and water. It has several industrial applications, including as a refractory material, in the production of magnesium metal, as a catalyst in chemical reactions, and as a source of magnesium ions in biological systems.

2.1.1 PHYSICAL PROPERTIES OF MgO

Magnesium oxide (MgO) is a chemical compound with a wide range of physical properties that make it useful in many different applications. MgO has a high melting point of 2,852℃ (5,166 °F), making it an ideal material for high-temperature applications. It also has a high boiling point of 3,600°C (6,500°F), which makes it an excellent material for use in refractory materials. The density of MgO is 3.58 g/cm^3, making it a relatively dense material. This high density makes it useful in applications where weight is not a concern, such as in construction materials. MgO is a hard and brittle material, with a Mohs hardness of 5.5. This makes it useful in abrasive applications, such as in grinding wheels and as a component in cutting tools.

2.1.2 CHEMICAL PROPERTIES OF MgO

Magnesium oxide is known for its remarkable chemical properties, which make it useful for a wide range of applications. One of the most notable chemical properties of MgO is its high reactivity. Magnesium oxide reacts vigorously with water, producing magnesium hydroxide ($Mg(OH)_2$) and releasing heat in the process. This reaction is highly exothermic and can result in a rapid increase in temperature, which makes MgO useful in applications where heat is required. For example, MgO is commonly used as a refractory material in high-temperature applications such as furnace linings and crucibles. Another important chemical property of MgO is its basicity. Magnesium oxide is a basic oxide, meaning that it reacts with acids to form salts and water. For example, when MgO is reacted with hydrochloric acid (HCl), magnesium chloride ($MgCl_2$) and water (H_2O) are produced:

$$MgO + 2HCl \rightarrow MgCl_2 + H_2O$$

This property makes MgO useful in a variety of industrial applications, including water treatment and acid neutralization.

Magnesium oxide also has excellent stability and is resistant to chemical attack from many substances. This makes it useful in applications where chemical stability is important, such as in the production of ceramics, glass, and refractory materials.

2.1.3 OPTICAL PROPERTIES OF MgO

MgO has a high refractive index, which means that it can bend light more than other materials with a lower refractive index. The refractive index of MgO varies with the wavelength of light, with values ranging from 1.71 to 1.84 in the visible region. This property makes it useful in optical applications such as lenses, prisms, and mirrors.

MgO is transparent in the visible and ultraviolet regions of the electromagnetic spectrum. It has a high transparency in the ultraviolet region, with a transmittance of over 90% in the range of 200-400 nm. This property makes it useful in applications such as UV filters and in the production of optical components for ultraviolet spectroscopy.

MgO exhibits birefringence, which means that it has different refractive indices for light polarized in different directions. This property makes it useful in applications such as polarizers, where polarized light needs to be separated into two beams. MgO has nonlinear optical properties, which means that its optical properties change when it is exposed to intense light. This property makes it useful in applications such as optical switches and frequency converters.

MgO exhibits luminescence when exposed to high-energy radiation such as X-rays or gamma rays. This property makes it useful in dosimetry applications, where it is used to measure the dose of radiation that has been absorbed by a material. MgO can exhibit fluorescence when doped with certain impurities. For example, when MgO is doped with chromium (Cr), it can emit green light when excited by a UV light source. This property makes it useful in optoelectronic applications such as lasers and LED lighting.

MgO exhibits absorption in the ultraviolet and visible regions of the spectrum. This property makes it useful as a pigment in white paints and as a UV-absorbing agent in sunscreen.

MgO exhibits electro-optic properties, which means that its optical properties can be altered by applying an electric field. This property makes it useful in various applications such as optical modulators and electro-optic switches.

2.2 CRYSTAL STRUCTURE

Magnesium oxide (MgO) has a face-centred cubic (FCC) crystal structure, also known as a rock-salt structure. In this structure, the magnesium cations ($Mg2^{2+}$) are located at the corners of the cube and the oxygen anions (O^{2-}) are located at the centre of each face of the cube. Each magnesium ion is surrounded by six oxygen ions, forming an octahedral coordination arrangement. Similarly, each oxygen ion is surrounded by four magnesium ions, forming a tetrahedral coordination arrangement. The lattice parameter, which is the distance between the centers of adjacent unit cells, is 4.213 Ångstroms (Å) at room temperature. The coordination number, which is the number of nearest neighbours of each ion, is 6 for both magnesium and oxide ions.

It is a highly symmetric structure with a high degree of packing efficiency, making it very stable and chemically inert. This crystal structure is very important in materials science, as MgO is a widely used ceramic material with a variety of applications, including as a refractory material in furnaces and crucibles, as an electrical insulator, and as a catalyst support.

2.3 METHOD USED

2.3.1 Co-precipitation Method

Co-precipitation is a standard synthesis method for preparation of metal oxide nanoparticles. In this method a salt precursor, commonly nitrate, chloride, or oxychloride, is dissolved in water and then the corresponding hydroxide is precipitated by addition of a base such as sodium hydroxide or ammonium hydroxide. Co-precipitation is a cost-effective and fast process and is easily implemented on a larger scale for industrial application. It is an efficient method for synthesizing nanomaterials without requiring hazardous organic solvents. However, there are some limitations such as control of size, shape, and crystalline and magnetic properties.

2.4 APPLICATIONS OF MgO NANOPARTICLES

Magnesium oxide (MgO) nanoparticles have a wide range of potential applications due to their unique properties, including high surface area, chemical stability, and biocompatibility. Here are some applications of MgO nanoparticles:

- Biomedical applications: MgO nanoparticles have antimicrobial and anticancer properties and can be used in drug delivery systems, medical imaging, and tissue engineering.

- Energy storage: It can be used as anode materials in lithium-ion batteries, which can improve battery performance and stability.

- Environmental remediation: It can remove heavy metals, organic pollutants, and other harmful substances from water and soil.

- Catalysis: It can be used as catalysts in a variety of chemical reactions, including the production of chemicals and pharmaceuticals.

- Flame retardants: It can be used as flame retardants in plastics and other materials to improve their fire resistance.

- Anti-corrosion coatings: It can be used as an additive in coatings to prevent corrosion.

- Gas sensors: It can be used as gas sensors for detecting and measuring gases in the environment.

- Antibacterial coatings: It can be used in coatings to prevent bacterial growth on surfaces.

- Food industry: It can be used as an additive in food packaging to extend shelf life and prevent bacterial growth

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- Water treatment: It can be used to remove impurities and improve water quality.

- Sunscreen: It can be used in sunscreen to provide protection from harmful UV radiation.

- Paints and coatings: It can be used in paints and coatings to improve durability and resistance to weathering.

- Additive in plastics: It can be used as an additive in plastics to improve their mechanical and thermal properties.

- Textile industry: It can be used as a flame retardant and an antibacterial agent in textiles.

- Construction industry: It can be used in concrete and other building materials to improve their strength and durability.

- Printing industry: It can be used as an additive in printing ink to improve adhesion and print quality.

- Optical applications: It can be used in optical coatings to improve light transmission and reflection.

- Cosmetics: It can be used in cosmetics as a filler or thickening agent.

- Agriculture: It can be used as a fertilizer additive to improve soil quality and crop growth.

- Bioremediation: It can be used to degrade organic pollutants in contaminated soil or water.

Overall, the properties of MgO nanoparticles make them promising candidates for a wide range of applications in various fields. However, further research is needed to fully understand their properties and potential uses.

2.5 FUTURE OPPORTUNITIES AND CHALLENGES

Nanotechnology may be the ultimate enabling technology, since it deals with the fundamental building blocks of matters. Almost every field will be deeply affected by the progress in nanotechnology. The most important impact of this nanotechnology revolution may be the new synergy among scientists, engineers, industrialists, entrepreneurs, financiers and economic development specialists. Scientists of yesterday are finding a need to understand Nano in order to perform their own research better. Nanotechnology creates both challenges and opportunities. In the research of Nano science and nanotechnology, one of the most important challenges would be growth, characterization and functionalization of nanomaterial and nanostructure: Nano design and simulation issues are just beginning to come out from the realms of human imagination. The future of nanotechnology rests in the hands of the current scientists that are ready and able to help guide this very young science into the next realm.

CHAPTER 3

PREPARATION AND CHARACTERIZATION TOOLS

3.1 CHEMICALS USED

$Mg(NO_3)_2$ as well as NaOH were used for synthesis of magnesium oxide nanoparticles. Magnesium nitrate is the inorganic nitrate salt of magnesium. It has a role as a fertilizer. It is an inorganic nitrate salt and a magnesium salt. It appears as a white crystalline solid. It produces toxic oxides of nitrogen if heated to decomposition. Used in pyrotechnics. Sodium hydroxide is also known as lye or soda , or caustic soda. At room temperature, sodium hydroxide is a white crystalline odourless solid that absorbs moisture from the air. It is a synthetically manufactured substance. When dissolved in water or neutralized with acid it releases substantial amounts of heat, which may prove sufficient to ignite combustible materials. Corrosive to metals and tissue. Used in chemical manufacturing, petroleum refining, cleaning compounds, drain cleaners.

3.1.1 PREPARATION

Co-precipitation method was used for synthesis of magnesium oxide nanoparticles. For this purpose, 0.2 M of $Mg(NO_3)_2$ as well as 2 M of NaOH was taken. Then concentration of $Mg(NO_3)_2$ were added to NaOH solutions and stirred for 60 minutes. The resulting components were separated by centrifugation and dried in the oven after being washed to remove the impurities. Then, magnesium hydroxide powder was calcinated at 450℃ in a furnace, and a white powder made up of magnesium oxide nanoparticles was obtained.

3.2 CHARACTERIZATION TECHNIQUES

Different techniques are available for the characterization of nanoparticles designed with specific properties and applications as per requirements.

3.2.1 X-RAY DIFFRACTION METHOD

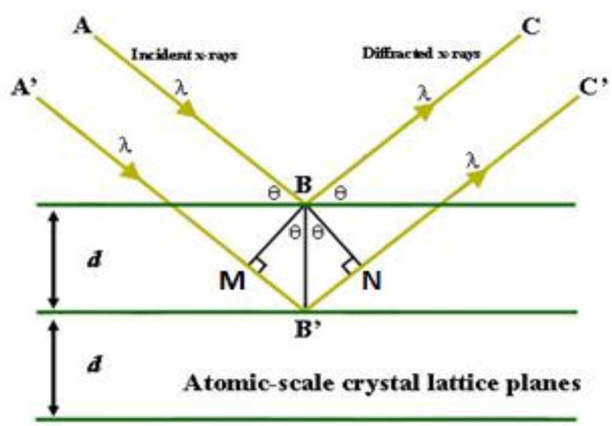
X-ray diffraction (XRD) technique is a precise and popular tool for determining the crystal structure of thin films. It yields complete information about the crystal structure, orientation, lattice constants, crystalline size and composition, defects and stress in the thin film. It requires no sample preparation and is essentially non-destructive

The wave nature of X-rays means that they are diffracted by the lattice of the crystal to give a unique pattern of peaks of "reflections" at differing angles and of different intensity, just as light can be diffracted by a grating of suitably spaced lines. The diffracted beam from atoms in successive planes cancels unless they are in phase, and the condition for this is given by Bragg's relationships. X-rays have wavelengths of the order of few angstroms (1A-0.1nm). This is the inter- atomic distance in crystalline solids, making X-ray the correct order of magnitude of diffraction of crystalline materials.

BRAGG'S LAW

In 1912, the scientists W.H Bragg and W.L Bragg put forward a model, which generates the condition for diffraction in a very simple way. They pointed out that through any crystal a set of equidistant planes can be drawn which passes through all the atoms of the crystal. In fact, a large number of such families of planes can be drawn. The planes of each family are separated from the other by a characteristic distance. These planes are called Bragg planes and their separation is called Bragg spacing equal to d. When a monochromatic beam of X-ray of wavelength 2, falls upon the atoms in the Bragg planes a wavelet of scattered radiation spread out from each atom in all directions.

This is shown in the figure.



Since X-ray are more penetrating than ordinary light, it is essential to consider the reflection at several such layers. At each layer, there is a partial reflection and the X-ray beam will be completely absorbed after penetrating a large number of layers. Now these reflected wavelets will reinforce themselves only when they meet. In the same phase, the condition for which is that the path difference between two such rays must be an integral multiple of wavelength.

In this figure, the wave falls on these planes at an angle θ , between the propagation direction of the incident beam and planes. The angle θ is known as glancing angle and reflection condition requires that $\theta = \theta'$

From the figure, the path difference is equal to MB'+B'N

The geometry of figure further gives

$$MB' + B'N = 2d\sin\theta \quad \text{—- (eq 1)}$$

Now condition for constructive interference becomes

$$2\,d\sin\theta = n\lambda \quad \text{—- (eq 2)}$$

Where n is the integer called order of reflection. The above equations (eq 1 & eq 2) together with the requirement $\theta = \theta'$ constitute Braggs law. If the X-ray wavelength is known, spacing d between adjacent Bragg planes in the crystal may be calculated.

PARTICLE SIZE DETERMINATION FROM XRD SPECTRUM

From the width of diffraction line, the average grain size of the film can be calculated using Debye-Scherer's formula

$$\text{Particle size,D} = \frac{K\lambda}{B\cos\theta}$$

Where, K is a constant which is nearly equal to 0.94.

B is the full width at half maximum measured in radians.

λ is the wavelength of X-ray

CRYSTAL STRUCTURE DETERMINATION FROM XRD SPECTRUM

For orthogonal crystals, the spacing between the lattice planes and lattice constants are related by the formula,

$$\frac{1}{d^2}=\frac{h^2}{a^2}+\frac{k^2}{b^2}+\frac{l^2}{c^2}$$

Where, d= Inter-planar spacing

a, b ,c- lattice constants

h, k, l - Miller indices of the planes

For cubic crystal structure, a=b=c,

$$\frac{1}{d^2}=\frac{h^2+k^2+l^2}{a^2}$$

CHAPTER 4

RESULTS AND DISCUSSIONS

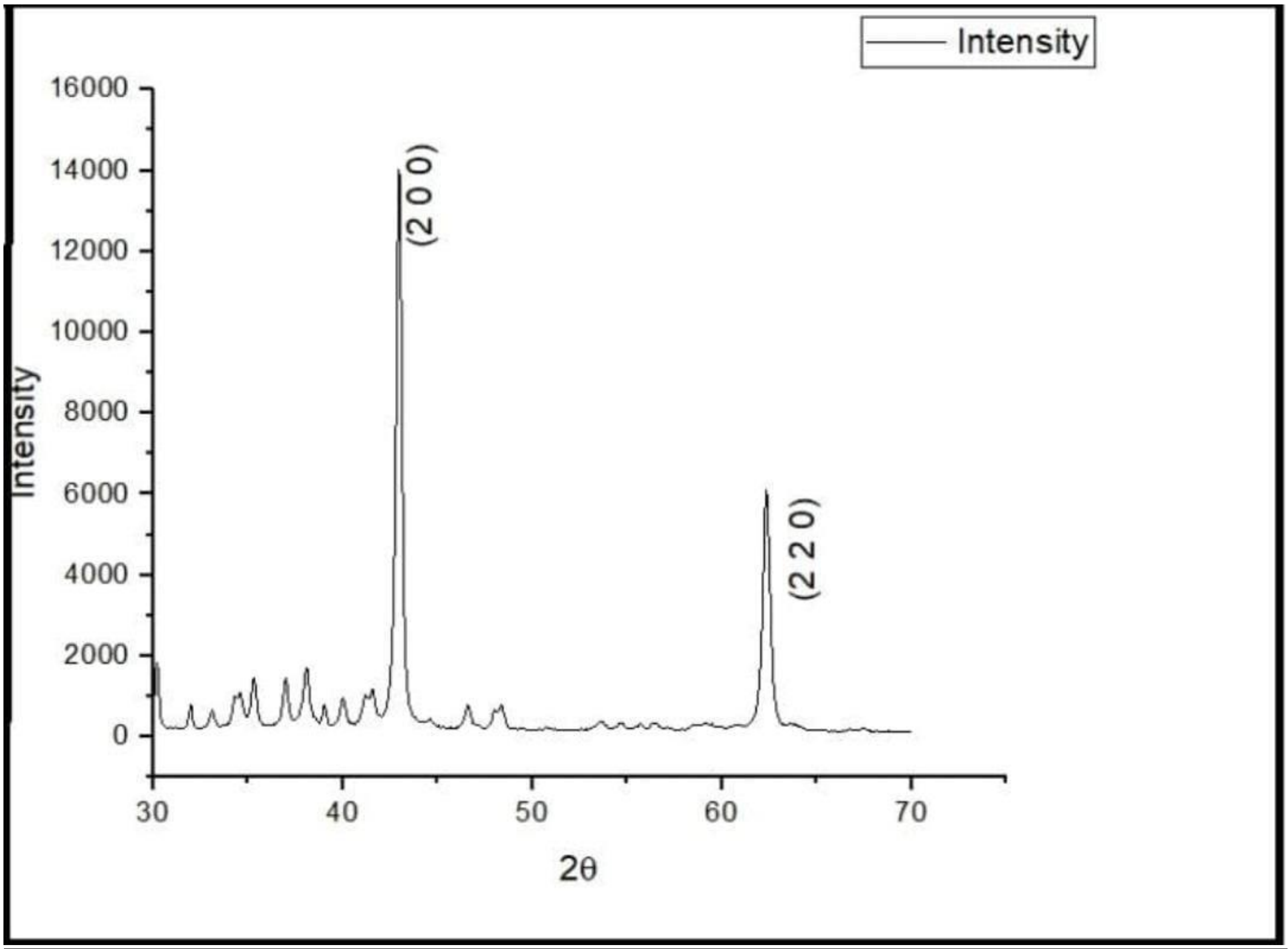
4.1 XRD ANALYSIS

X-Ray diffraction is a non-destructive analytical technique which can yield the unique fingerprint of Bragg reflections associated with a crystal structure sensitive to ordering over tens of nanometres. It uses x-rays to investigate and quantify the crystalline nature of materials by measuring the diffraction of x-rays from the planes of atoms within the material. It is sensitive to both the type and relative position of atoms in the material as well as the length scale over which the crystalline order persists. It can, therefore, be used to measure the crystalline content of materials ;identify the crystalline phases present, determine the spacing between lattice planes and the length scales over which they persist; and to study preferential ordering and epitaxial growth of crystallites.

Analysis of the diffraction pattern allows the identification of phases within a given sample. With that achieved ,it may be possible to quantify each phase present ,the crystallite of a sample ,the crystal structure and their lattice parameters ,crystallite size and strain. All information provides vital information in material characterization and quality control.

Magnesium oxide nanoparticles prepared in the laboratory are characterized using XRD technique and the resultant XRD data is provided below. The obtained 2θ values are found to be coinciding with the standard JCPDS card number 75-1525 of Magnesium oxide nanoparticles.

4.1.1 XRD PATTERN OF MAGNESIUM OXIDE NANOPARTICLES



4.1.2 PARTICLE SIZE DETERMINATION

The particle size of nanoparticle can be calculated using Debye-Scherrer equation:

$$\textbf{Particle size,D=}\ \frac{K\lambda}{B\cos\theta}$$

Where K is constant which is nearly equal to 0.9

B is the full width at half maximum measured in radians.

λ is the wavelength of X-ray.

Using XRD data in the Debye-Scherrer formula, the particle size of magnesium oxide are calculated as follows:

Standard 2θ (Degree)	Observed 2θ (Degree)	θ (Degree)	θ (Radian)	B (Degree)	B (Radian)	Particle Size D(nm)
42.94	42.99	21.495	0.375	0.34844	0.00608	23.818
62.25	62.342	31.171	0.5440	0.44072	0.00769	18.832

Hence average particle size, **D = 21.325 nm**

Calculation

Taking, 2θ = 42.99

θ = 0.375 radian

B = 0.00608

= 1.54060 A°

Therefore $D = \frac{0.9\,\lambda}{B\,Cos\,\theta}$

$$= \frac{0.9 \times 1.54060 \times 10^{-10}}{0.00608 \times Cos\,(0.263)}$$

$$= 23.818 \text{ nm}$$

4.1.3 LATTICE PARAMETER CALCULATIONS

The crystal structure of magnesium oxide nanoparticles are determined from XRD spectrum analysis and it was found that magnesium oxide nanoparticles has got a face- centred cubic structure with lattice parameters a=b=c and α=β=γ=90°.Lattice constant "**a** "can be calculated by

$$a = \sqrt{(h^2 + k^2 + l^2)d^2}$$

Where d is the inter-planar spacing

h, k , l are miller indices

Calculated Lattice constant for each d is tabulated below:

d	h	k	L	Calculated a (A°)
2.102	2	0	0	4.2045
1.488	2	2	0	4.2089

Mean lattice parameter, **a = 4.2067 A°**

Standard lattice parameter, a = 4.195 A°

Therefore lattice parameter obtained here is in close agreement with the standard value .

CONCLUSION

MgO nanoparticles were successfully synthesized using co- precipitation method. The structural characterization of MgO nanoparticles was done through XRD analysis. Average particle size and lattice parameter were also calculated. From XRD analysis average crystallite size of the sample was determined as **21.325 nm**. The lattice parameter was found to be of value **4.2067 A°** which is in close agreement with the standard values.

REFERENCES

1. Hindawi, Journal of Nanotechnology Volume 2019, Article ID 6063832,

2. Metal Oxide Nanoparticles -Marcos Fernández-Garcia, José A. Rodriguez To be published in "Nanomaterials: Inorganic and Bioinorganic Perspectives". October 2007, Chemistry Department, Brookhaven National Laboratory

3. The Synthesis and Characterization of Gold and Silver Nanoparticles in Mathew Wynn Materials Engineering Department California Polytechnic State University, San Luis Obispo Advised by Dr. Katherine C. Chen.

4. A facile one step solution route to synthesize cuprous oxide Nano fluid(Regular paper)-Shenoy U, Sandhya and Shetty A Nityananda -Department of Chemistry National Institute of Technology, Karnataka, Surathkal, Mangalore, Karnataka, India.

5. L. Castro, M. L. Blázquez, J. á. Muñoz, F. G. González, and A. Ballester, "Mechanism and applications of metal Nano-particles prepared by bio-mediated process," Reviews inAdvanced Sciences and Engineering, vol. 3, no. 3, pp. 199-216,2014.

6. E. M. Hotze, T. Phenrat, and G. V. Lowry, "Nanoparticle aggregation: challenges to understanding transport and re- activity in the environment," Journal of Environment Quality, vol. 39, no. 6, pp. 1909-1924, 2010

7. K. G. Rao, C. H. Ashok, K. V. Rao, and C. S. Chakra, "Structural properties of MgO nanoparticles: synthesized by co-precipitation technique," International Journal of Science and Research, vol. 3, no. 12, pp. 43-46, 2014.

8. M. Sundrarajan, J. Suresh, and R. R. Gandhi, "A comparative study on antibacterial properties of MgO nanoparticles pre- pared under different calcination temperature," Digest journal of nanomaterial and bio structures, vol. 7, no. 3, pp. 983-989, 2012.