SUDAN UNIVERSITY OF SCIENCE AND TECHNOLOGY

College of post graduate Studies

# Mg Doped on ZnO to Investigate the Effect of Mg Ions on optical properties and bandgap of ZnO Nano-particle

# إضافة الماغنسيوم لأكسيد الزنك للتحقق من تأثير ايونات الماغنسيوم على الخصائص البصرية وفجوة الطاقة لجسيمات اكسيد الزنك النانوية

Acomplementary research Submitted for partial fulfillment of the requirements for the Degree of M.Sc. in Physics

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**November 2015**

## الآية

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صدق الله العظيم

الأنبياء: ٤٧

## *Dedication*

**Special dedication to my parents, thanks for your care,**

**kindness and your great love**

**To my brothers and sisters**

**To my close friends and colleagues**

# Acknowledgements

First, thanks god for giving me power to complete this research

Then, I have to thank my parent, whom continue to grow, learn and develop and whom have been a source of encouragement and inspiration to me through my life .

I would like sincerely to thank my supervisor, Dr. faiz Mohamed badr , for his grate patient, constructive criticisms, and myriad useful suggestion apart from invaluable guidance and support through this research .

To all my friends, thank you for your understanding and encouragement .your friendship makes my life a wonderful experience. I cannot list all the names here you are always in my heart .

# Abstract

In this study, the optical (absorption coefficient and transparency) properties and the energy band of Zinc Oxide nano particles doped with magnesium ion were investigated within different weight percent namely (0.00 , 0.05 and 15% of weiht) was synthesized , the ZnOnano particles was prepared using sol–gel method. A UV-VIS spectrophotometer used to investigate the absorption coefficient and transparency of ZnO nanoparticles with each weight percent adding of magnesium ion, The results indicates that the transmittance has a tendency to decrease with Mg progressed, , the results also show that Absorption coefficients in the UV region significantly increased with Mg progress and due to tauc equation the bandgap of ZnO nanoparticle can be change as Mg progressed.

# المستخلص

في هذه الدراسة تم التحقق من الخواص البصرية (النفاذيه ومعامل الامتصاص) والمجال المحظور لجسيمات أكسيد الزنك النانويه المضاف إليها أيونات المغنيسيوم بنسب مختلفة ( 0.00 , 0.05 , 0.15 ) من الوزن %Mg-ZnO من ثم . حضر أكسيد الزنك النانوي بطريقه السل-جيل. استخدم مطياف الأشعة فوق البنفسجية للتحقق من الخواص البصرية للمركب. أوضحت النتاج أن النفاذية تتغير معزيادة كميه المغنيسيوم المضاف وان معامل الامتصاص يزداد بصوره واضحة عند زيادة المغنيسيوم كما لوحظ أن قيم المجال المحظور المتحصل عليها من النتاج تزيد بزيادة النسبة المضافة من المغنيسيوم . (باستخدام معادله تاوك tauc equation )

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# Chapter One
# Background of study

## 1.1 Introduction:

Metal oxides play a very important role in many areas of physics and materials science. The metal elements are able to form a large diversity of oxide compounds. These can adopt a vast number of structural geometries with an electronic structure that can exhibit metallic and semiconductor character. In technological applications, oxides are used in the fabrication of microelectronic circuits, sensors, piezoelectric devices, fuel cells, and as catalysts[1,2].

Zink oxide one of oxides which is a very promising material for semiconductor device applications [3-7], It has a direct and wide band gapof 3.37 ev[8-11] and a large free-exciton binding energy about60 mev in a semiconductor [8-10] so that excitonic emission processes canpersist at or even above room temperature[12-13] ,the availability of high-quality large bulk single crystals, the strong luminescence demonstrated in optically pumped lasers and the prospects of gaining control over its electrical conductivity have led a large number of groups to turn their research for electronic and photonic devices to ZnO in its own right,The high electron mobility, high Thermal conductivity, wide and direct band gap and large excision binding energy make ZnO suitable for a wide range of devices, including transparent thin-film transistors, photo detectors, light-emitting diodes and laser diodes that operate in the blue and ultraviolet region of the spectrum . The band gap of ZnO can be controlled via divalent substitution onthe cation site. The band gap can be decreases by substituting Cd on Zn site, and, on the other hand, substituting Mg on Zn site increases the band gap [14].. It is possible to obtain a wide band gap ternary ZnMgO alloy by doping ZnO with a suitable ratio of Mgwhich has a band gap of 7.8 eV.altering the band gap will affect the optical behavior as well as other properties.

## 1.2 Aim of this work:

**1-**To synthesize $Mg_xZn_{1-x}O$ (x=0.00 , 0.05 ,0.15) .

**2-**To study the optical properties of Mg-ZnO and investigate the effect of divalent element Mg in energy bandof ZincOxide.

## 1.3 Outlines of thesis:

This thesis consist of four chapters, chapter one is intended to the background of study which contains introduction, the objective of the research, and the layout ,then chapter twois review of theoretical background concerning the zinc oxide material and the techniques which used to investigate the properties of materials , mainly X-ray diffraction, Bragg's law , infrared spectroscopy , ultraviolet-visible spectroscopy an scanning electron microscopy,chapter three stated for the experiment and method, finally chapter four is for the result and discussion.

## 1.4 Literature review:

### 1.4.1 Effects of Mg Incorporation on Microstructure and Optical Properties of ZnO Thin Films Prepared by Sol-gel Method

*Rui Ding*1), *Chunxiang Xu*1)*y*, *Baoxiang Gu*1), *Zengliang Shi*1), *Haitao Wang*2), *Long Ba*2) *and Zhongdang Xiao*2)1) Advanced Photonics Center, School of Electronic Science and Engineering, Southeast University, Nanjing *Rui Ding*1), *Chunxiang Xu*1)*y*, *Baoxiang Gu*1), *Zengliang Shi*1), *Haitao Wang*2), *Long Ba*2) 210096, China 2) State Key Laboratory of Bioelectronics, Southeast University, Nanjing 210096, China

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Well-crystallized MgZnO alloy thin ¯lms with hexagonal wurtzite structure were fabricated by sol-gel method.
With the band gap increases, the surface roughness and the grain size reduces. It is worth noting that the intensity of the band-edge luminescence of Mg doped ¯lms enhances with the increase of the Mg content. The microstructure and photoluminescence mechanism have been discussed based on X-ray di®raction patterns, atomic force microscopy images, ultraviolet-visible absorption spectra, photoluminescence spectra and Fourier transform infrared spectra.

**1.4.2 Bandgap Alteration of Transparent Zinc Oxide Thin Film with Mg Dopant.**

M. Salina and R. Ahmad (NANO ElecTronic Centre, Faculty of Electrical Engineering, UniversitiTeknologi MARA, 40450 Shah Alam, Selangor, *Malaysia*) , A. B. Suriani (NANO SciTech Centre, Institute of Sciences, UniversitiTeknologi MARA, 40450 Shah Alam, Selangor, Malaysia) and M. Rusop(NANO ElecTronic Centre, Faculty of Electrical Engineering and NANO SciTech Centre, Institute of Sciences, Universiti Teknologi MARA, 40450 Shah Alam, Selangor, Malaysia)
Received November 3, 2011; Revised January 5, 2012; Accepted January 21, 2012.
They have successfully demonstrated a bandgap alteration of transparent zinc oxide (ZnO) thin film with Mg dopant by using sol-gel spin coating technique. By increasing the dopant from 0 to 30 atomic percent (at.%), a decrement value in the cutoff is observed, where the absorption edge shifts continuously to the shorter wavelength side, towards 300 nm. This resulted in a significant bandgap increment from 3.28 to 3.57 eV. However, the transmittance of the thin film at 350-800 nm gradually

downgraded, from 93 to 80 % which is most probably due to the grain size that becomes  bgger, and it also affected the electrical properties.

# Chapter Two

# Theoretical Background

## 2.1 Introduction:

This chapterconsist of the general concepts of the nanoparticle materials which werebriefly reviewed, properties of zinc oxide, properties of magnesium, synthesize method of nano material and technique which used to investigate the properties of materials specially ultraviolet-visible spectroscopy method which used in this research .

First its necessary to consider the general concepts relate to the nano-size objects, a nano-objects is a physical objects differing appreciably in properties from the corresponding bulk material at having at least 1nm dimension (not more than 100 nm ) . Nanomaterials are those materials whose key physical characteristics are decade by the nano-objects they contains.

Nanotechnology is the technology dealing with both single nano-objects materials and devices base on them , and with processes that take place in the nanometer range . In the emerging field of nanotechnology, a goal is to make nanostructures with special properties with respect to those of bulk or single particle species. Oxide nanoparticles can exhibit unique physical and properties due to their limited size and a high density of corner or edge surface sites.

Particle size is expected to influence three important groups of basic properties in any material. The first one comprises the structural characteristics, namely the lattice symmetry and cell parameters [13]. Bulk oxides are usually robust and stable systems with well-defined crystallographic structures. However, the growing importance of surface free energy and stress with decreasing particle size must be considered: changes in thermodynamic stability associate with size can induce modification of cell parameters and/or structural transformations and in extreme cases the nanoparticle can disappear due to interactions with its surrounding environment and a high surface free energy. In order to display structural stability, a nanoparticle must have a low surface free energy. As a consequence of this requirement, phases that have a low stability in bulk materials can become very stable in nanostructures.

The second important effect of size is related to the electronic properties of the oxide. In any material, the nanostruture produces the so-called quantum size or confinement effects which essentially arise from the presence of discrete, atom-like electronic states. From a solid-state point of view, these states can be considered as being a superposition of bulk-like states with a concomitant increase in oscillator strength[15]. Theoretical studies for oxides show a redistribution of charge when going from large periodic structures to small clusters or aggregates which must be roughly considered to be relatively small for ionic solids while significantly larger for covalent ones[16,17,18,19.20,21]. The degree of ionicity or covalency in a metal oxygen bond can however strongly depend on size in systems with partial ionic or covalent character; an increase in the ionic component to the metal-oxygen bond in parallel to the size decreasing has been proposed[22]. Structural and electronic properties obviously drive the physical properties of the solid.

The third group of properties influenced by size in a simple classification . In their bulk state, many oxides have wide band gaps and a low reactivity[23]. A decrease in the average size of an oxide particle do in fact change the magnitude of the band gap[24,25],with strong influence in the conductivity [26,27].Surface properties such as energy levels , electronic structure , and reactivity can be quite different from interior state , an give rise to quite different material properties .

## 2.2 Zinc Oxide nanoparticles:

### 2.2.1 Brief overview of ZnO

Today, when the world is surmounting on the roof of technology and electronics, mostly dominated by compatible electronic equipments and thereby creating the need for materials possessing versatile properties. The type of material a very common category of material comes out that is semiconductor. Germanium get famous due to possession of property like low melting point and lack of natural occurring germanium oxide to prevent the surface from electrical leakage where as silicon dominates the commercial market for its better fabrication technology and application to integrated circuits for different purposes .As time passes on, the rapid growing world demands a material that should possess inherent properties like larger band gap, higher electron mobility as well as higher breakdown field strength. So on making investigation about such a material the name of compound comes out is “Zinc Oxide” which is a wide gap semiconductor material very well satisfying the above required properties also Zinc oxide possessed many versatile properties for UV electronics, spintronic devices and sensor applications. Zinc oxide is an inorganic compound with the formula ZnO. It usually appears as a white powder, nearly insoluble in water. The powder is widely used as an additive into numerous materials and products including plastics, ceramics, glass, cement, rubber, lubricants, paints, ointments, adhesives, sealants, pigments, foods (source of Zn nutrient), batteries, ferrites, fire retardants, etc. ZnO is present in the Earth crust as mineral zincates; however, most ZnO used commercially is produced synthetically.

The research on ZnO is catching fire right from the beginning of 1950, with a number of reviews on electrical and optical properties like N-type conductivity, absorption spectra and electroluminescence decay parameter [28].

### 2.2.2 Fundamental properties of ZnO:

Zinc oxide crystallizes in three forms: hexagonal wurtzite, cubic zincblende, and the rarely observed cubic rock salt, fig (1). The wurtzite structure is most stable and thus most common at ambient conditions. The zincblende form can be stabilized by growing ZnO on substrates with cubic lattice structure. The hexagonal and zincblendeZnO lattices have no inversion symmetry (reflection of a crystal relatively any given point does not transform it into itself). This and other lattice symmetry properties result in piezoelectricity of the hexagonal and zincblendeZnO, and in piezoelectricity of hexagonal ZnO. The lattice constants are a=3.25Å and c = 5.2 Å; their ratio c/a ~ 1.60 is close to the ideal value for hexagonal cell c/a = 1.633 .

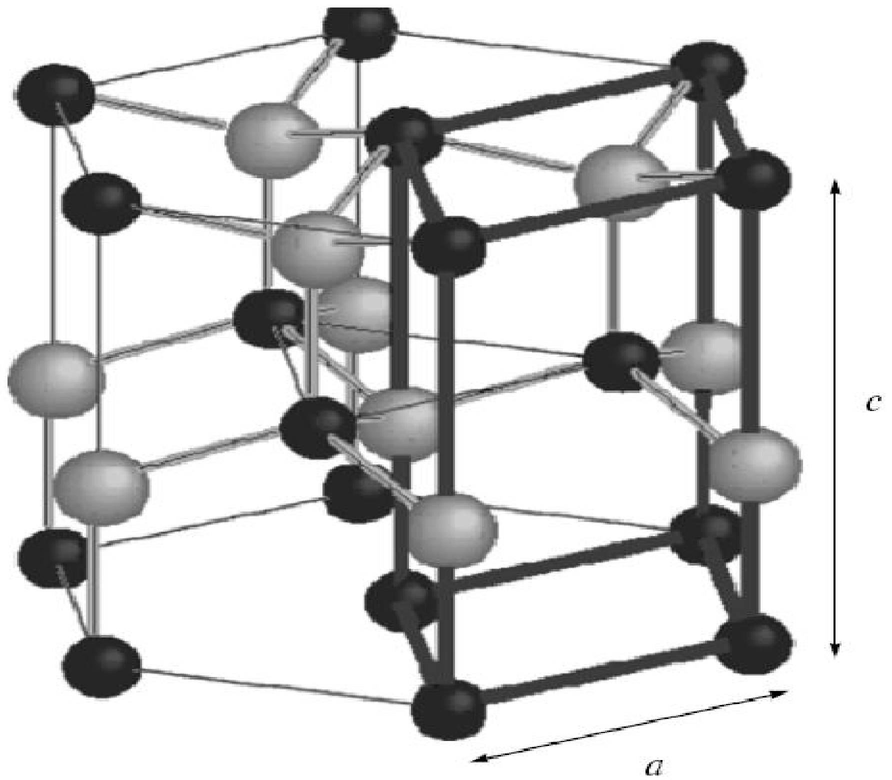
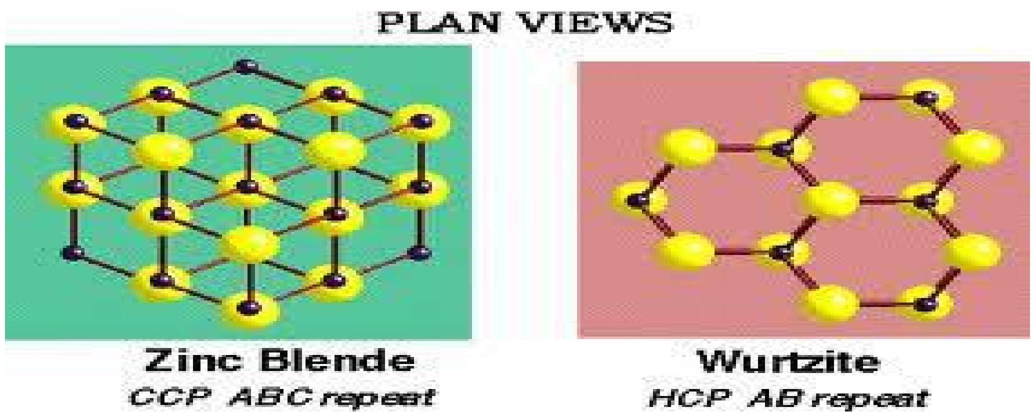



**Fig. 1.** Primitive cell (thick lines) and hexagonal prism of the wurtzite structure of ZnO: (*a*) and (*c*) are the lattice constants (black and white spheres denote Zn and O, respectively).




Figure(2-2) type of zinc oxide structure

ZnO is a direct band semiconductor and a transparent conductive material. ZnO films are transparent in the wavelength range of 0.3 and 2.5 μm, and plasmaedge lies between 2 and 4 μm depending on the carrier concentration. It is well known that a shift in the band gap edge appears with an increase in the carrierConcentration. This shift is known as Burstein-Moss shift. Optical transitions in ZnO have been studied by a variety of experimental techniques such as optical absorption, transmission, reflection, spectroscopic.ZnO has a direct band gap of 3.37 eV with excitonic energy of 60 meV in a semiconductor. Hall mobility in ZnO single crystal is on the order of $200 cm^2V^{-1}s^{-1}$ at room Temperature[8].

## 2.3Magnesium (doping material) :

Magnesium only occurs naturally in combination with other elements , where it invariably has a +2 oxidation state. the free element can be produce artificially and is highly reactive. It exhibits a rock salt structure like oxides of other alkaline earth metals. In its bulk state, MgO is a highly ionic compound and a wide band gap (~ 7 eV)insulator. For small nanoparticles of MgO, a reduction in the band gap could be measuredby using optical absorption techniques. And the effects of the electrostatic Madelungpotential could not be as strong as those in bulk MgO

Mg is the most popular doping material as the ionic radii

Of Mg2+ and Zn2+ are nearly equal and so, this resulted in a very little lattice distortion when Zn ion is replaced by Mg ion [17,18].

## 2.4 synthesize method :

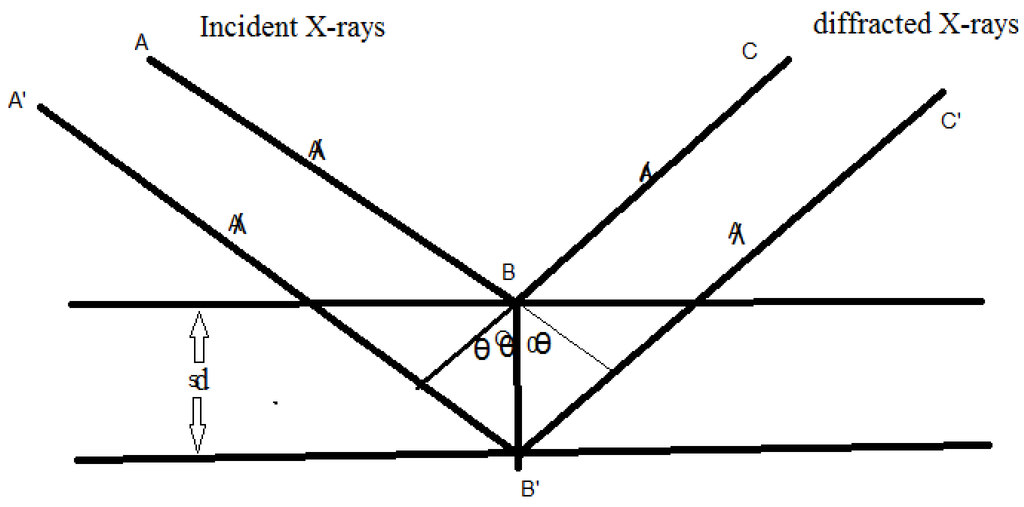
Various methods have been used to prepare MgZnO nanoparticle, among which magnetron sputtering, pulsed laser deposition (PLD) [23-28]pyrolysis and hydrothermal synthesis and sol-gel are common. The samples which are prepared by sol-gel technique are the most promising one for a low cost, long length, and low temperature process. This method is also used to prepare the complex oxide composition with high homogeneity and versatility in coating different substrate materials [29, 30, and 31].

The **sol-gel** process is a method for producing solid materials from small molecules. The method is used for the fabrication of metal oxide, especially the oxides of silicon and titanium. The process involves conversion of monomers into a colloidal solution (*sol*) that acts as the precursor for an integrated network (or *gel*) of either discrete particles or network polymers. Typical precursors are metal alkoxides.In this procedure, the 'sol' (or solution) gradually evolves towards the formation of a gel-like diphasic system containing both a liquid phase and solid phase whose morphologies range from discrete particles to continuous polymer networks. In the case of the colloid, the volume fraction of particles (or particle density) may be so low that a significant amount of fluid may need to be removed initially for the gel-like properties to be recognized. This can be accomplished in any number of ways. The simplest method is to allow time for sedimentation to occur, and then pour off the remaining liquid.Centrifugation can also be used to accelerate the process of phase separation.Removal of the remaining liquid (solvent) phase requires a drying process, which is typically accompanied by a significant amount of shrinkage and densification. The rate at which the solvent can be removed is ultimately determined by the distribution of porosity in the gel. The ultimate microstructure of the final component will clearly be strongly influenced by changes imposed upon the structural template during this phase of processing.Afterwards, a thermal treatment, or firing process, is often necessary in order to favor further polycondensation and enhance mechanical properties and structural stability via final sintering, densification and grain growth.

## 2.5Principle of X-Ray diffraction (XRD)

X ray can be diffracted in a manner similar to that of the visible light by a ruled grating.

In order to obtain diffraction spectrum the crystalline sample is strucked by an x-ray beam at some angle theta, apportion of the beam scattered by the atoms on the surface, fig (2-3)




**Figure(2-3)Schematic of  X-ray diffraction phenomena**

The un scattered portion of the beam penetrates to the  next layer of atom where diffraction of the beam is again scatter and the rest passes to the next layer an so fourth , the scattering effect produces diffraction of the beam of  X-ray radiation .

Consider multiple planes ,ifrays A andA' are scattered by B and B'

and the path difference between ABC an A'B'C' which shown at fig (2-3) given by equation below

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

The ray A and A' will completely in phase with each other if the difference is equal to whole number of wavelength, ie

$$n\lambda = 2d \sin\theta \qquad (2\text{-}2)$$

where n = 1,2,3,etc…., and θ is the angle at which crystal plane is incline to the incident beam , if the above condition is not satisfied , instructive interference occurs .

this relation was rive by W.L Bragg , and is called Bragg's law .

## 2.6 Scherer's formula:

the crystallite size of MgxZn1-xO present in the investigate was base on X-ray diffraction line broadening an calculate by using Scherer's equation (35) .

$$D = \frac{B\lambda}{\beta cos\theta} \qquad (2\text{-}3)$$

WhereD is the average crystallite size of the phase under investigation, B is scherrer constant (32), $\lambda$ is the wave length of X-ray beam use .$\beta$is the full with at half maximum (FWHM) of diffraction and θ is the Bragg's angle.

## 2.7 Fourier transforms infrared spectroscopy (FT-IR)

Infrared is a common vibrational spectroscopy technique useful for determination of compounds functional groups. Compounds having a covalent bon , whether organic or inorganic absorb various frequencies of electromagnetic radiation in the infrared region of the electromagnetic spectrum . in terms of wave numbers, the vibrational infrared extend from about 4000 to 400 $cm^{-1}$ . in infrared absorption process molecule are existed to a higher energy state when they absorb infrared radiation. Radiation in this energy range correspond to the range encompassing the stretching an bending vaibrational frequencies of the bon in most covalent bon .as for many harmonic oscillator , when a bond vibrates , its energy of vibration continuously an periodically changing from kinetic to potential energy an back again . the total amount of energy is proportional to the frequency of vibration. (4,8)

$$E_{osc} \propto h\gamma_{osc} \quad (2.4)$$

The natural frequency of vibration of abond is given by the equation

$$v = \frac{1}{2\pi c}\sqrt{\frac{k}{\mu}} \qquad (2\text{-}5)$$

Which is drive from hook's law for vibrating spring . K represents the force constant of the spring and$\mu$ represent the reduce mass of the system. FTIR spectroscopy is a preliminary test to detect both organic and inorganic molecules in a compound.

### 2.7.1 Modes of vibration :

Molecules with vibrational frequencies, for nonlinear molecule with atoms, the number of vibration modes is (3n-6) corresponding to the

Cartesian coordinates, where n is the number of atoms in the molecule. There are tow different types of virational modes. vibrational either involve a change in bond length (stretching) or bond angle .

## 2.8 Ultraviolet-visible spectroscopy :

The instrument use in ultraviolet spectroscopy is called a UV-VIS spectrophotometer. It measure the intensity of light passing through a sample (I), an compare it to the intensity of light before it passes through the sample(Io).the ratio I/Io is called the transmittance , andit's usually expresses as a percentage (%T) . The absorbance, A is base on the transmittance.

$$A = -\log(T(100\%)) \qquad (2\text{-}6)$$

The uv-visible spectrophotometer can also be configure to measure reflectance .in this case, the spectrophotometer the intensity of light reflected from a sample ($I_R$),and compares it to the intensity of light incident onthe sample ($I_i$). The ratio $I_R/I_i$ is called the reflectance , and usually expresses as percentage(%R).

Ultraviolet-visible spectroscopy or ultraviolet-visible spectrophotometry (UV-Vis or UV/Vis) refers to absorption spectroscopy or reflectance spectroscopy in the ultraviolet-visible spectral region. This means it uses light in the visible an adjacent (near-uv and near-infrared [NIR] range). The absorption or reflectance in the visible range directly affects the perceive color of the chemicals involve. In this region of the electromagnetic spectrum, molecules undergo electronic transition, this technique is complementary to fluorescence spectroscopy, in that fluorescence deals with transition from the excite state to the ground state, while absorption measures transition from the ground state to the excite state .

## 2.9 Beer-lamberts law :

The method is most often use in a quantative way to determine concentrations of an absorbing species in solution, using the beer-lamberts law;

$A = \log_{10} (Io/I) = \epsilon c L$ (2.3)

Where A is the measure absorbance, in absorbance unit (AU) ,Io is the intensity of the incident light at a given wavelength, I is the transmitted intensity , L is the path length through the sample an c is the concentration of the absorbing species. For each species an wavelength, ϵ is a constant known as the molar absorptivity or extinction coefficient. This constant is fundamental molecular property in a given solvent, at a particular temperature and pressure. The absorbances an extinction ϵ are sometimes define in terms of the natural logarithm instead of the base -10 logarithm.

The beer-lamberts law is useful for characterizing many compounds but does not hold as a universal relationship for the concentration absorption of all substances. A 2n order polynomial relationship between absorption an concentration is sometimes encountered for very large, complex molecules such as organic dyes.

# Chapter three
# Experimental

## 3.1 Materials and Equipments :

- Methanol (CH3OH) .
- Triethanolamine (TEA)N(CH2CH2OH)3(molecular weight =149.5), supplied by chemical laboratory–SUDAN UNIVERSITY OF SCIENCE AND TECHNOLOGY.
- Zinc acetate dehydrate $Zn(CH_3coo)_2.2H_2O$(molecular weight =219.51) supplied by chemical laboratory – Khartoum university.
- Magnesium acetate tetra hydrate$Mg(CH_3Coo)_2.4H_2O$ (molecular weight =214.5) supplied by chemical laboratory-Karary university).
- Magnetic stirrerFigure (3-1).

Is a laboratory device that employs a rotatingmagnetic field to cause a stir bar immersed in a liquid to spin very quickly, thus stirring it. A heating element whose power may range from a few hundreds to a few thousand watts can also be incorporated to the stirrer to allow the reaction flask to be heated and stirred at the same time.

- Beaker and conical flaskFigure (3-2).
- Thermometer (0-100) C.
- Oven.

- UV-1800 ( UV-Visible ) SpectrophotometerFigure (3-3) , supplied by Shimadzu, at the central laboratory of Khartoum university .

The UV-1800 UV-VIS spectrophotometer achieves a resolution of 1 nm, the highest in its class, in a compact design. Offering an array of user-friendly features, the UV-1800 can be used either as a stand-alone instrument or as a PC-controlled instrument. Equipped with a variety of measurement modes and numerous functions as standard in a stand-alone instrument, the UV-1800 enables you to perform a range of applications, including photometric and protein quantitation.

**Photometric Mode**

Measures the absorbance or transmittance at a single wavelength or at multiple (up to eight) wavelengths.

**Spectrum Mode**

Obtains sample spectra using wavelength scanning. Changes in the sample can be tracked using repeated scans.

**Quantitation Mode**

Generates a calibration curve from standard samples, and uses it to calculate the concentrations of unknown samples.

**Kinetics Mode**

Measures the change in absorbance as a function of time, and thereby obtains enzymatic activity values **.**

**Time-Scan Mode**

Measures the change in absorbance, transmittance, or energy as a function of time .

**Multi-Component Quantitation Mode**

Separately quantitates up to eight components mixed in a single sample. Pure components or mixtures of components can be used as standard samples.

**Biomethod Mode**

Capable of analyzing DNA and proteins .


**Figure(3.1)magneticstirrer.Figure(3.2)Beaker and conicalflask**

**Figure (3.3) UV-1800 ( UV-Visible ) Spectrophotometer**

## 3.2 Methodology:

The MgZnO thin films were prepared by sol-gel method. At first, $Zn(CH_3COO)_2.2H_2O$ and $Mg(CH_3COO)_2.4H_2O$ were dissolved together in methanol ($CH_3OH$) at room temperature, and thenthe triethanolamine ($HN(CH_2CH_2OH)_3$, TEA) wasadded drop wise to the solution as the stabilizer. The totalconcentration of the metal ions was controlled at0.5 mol/L in the solution, and the molar ratio ofthe DEA to the total metal ions was 1:1. The $Mg^{+2}$concentration was chosen as 0.00, 0.05and 0.15mol/L for different samples (A, B, C), respectively. The solution was stirred for about 1 h at $60^0$±C by magnetic stirrer until a clear and transparent solutionwas obtained and then the solution cooled in the air for 1 hour until white sedimentsappear. Thesolution obtained was immediately pre-heated at $150^0$±Cfor 1 h to evaporatethe solvent and other organic component, this process change the solution to gil-like homogeneous phase.Annealing process tookplace at $300^o$ Cfor 1 hours.Finally, thesamples weredried in air for 20 hours andchanged to powder.

**Zinc acetate dehydrate and Magnesium acetate tetra hydrate**

**Dissolve in methanol**

**Add TEA**

**Mixed with magnetic stirrer for 1 hours at $60^0$C**

↓

**transparent solution**

↓

**solvent evaporated for 1 hour at $150^0$C**

↓

**Annealing 250 – $300^o$ C**

↓

**dried in air for 20 hours**

↓

**MgZnO (powder)**

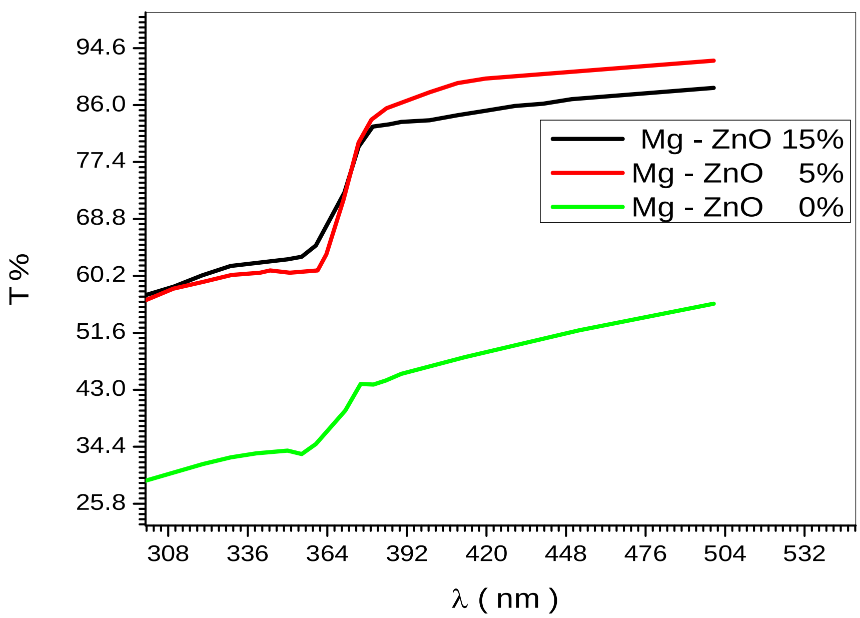
**Fig ( 3.4) Flow chart for the preparation of MgZnO powder**

# Chapter Four

# Results and Discussions

Using the UV-Visible Spectrophotometer the synthesized ZnOnano structure samples were characterized and the result below obtained.

## 4.1 Transmittancy:




**Figur(4.1) Relation btween wave length(nm) and transmition(%).**

The figure shows the optical transmittance spectra of $Mg_xZn_{1-x}O$ (0.0<x<0.15) nanoparticle in the wavelength range between 300 to 540 nm .The transparency properties samplesB and Care more than 80 % and sample Ais above 45% at a visible wavelength , It is observedthat the transmittance has a tendency to decrease with Mg progressed.

In addition the figure shows that the synthesized nano particles samples had a very effective UV blocking effect.The low transmission in the range 300-360(nm) indicating that the Mg-ZnOnano particles have a high shielding effect.

## 4.2Absorption coefficient:

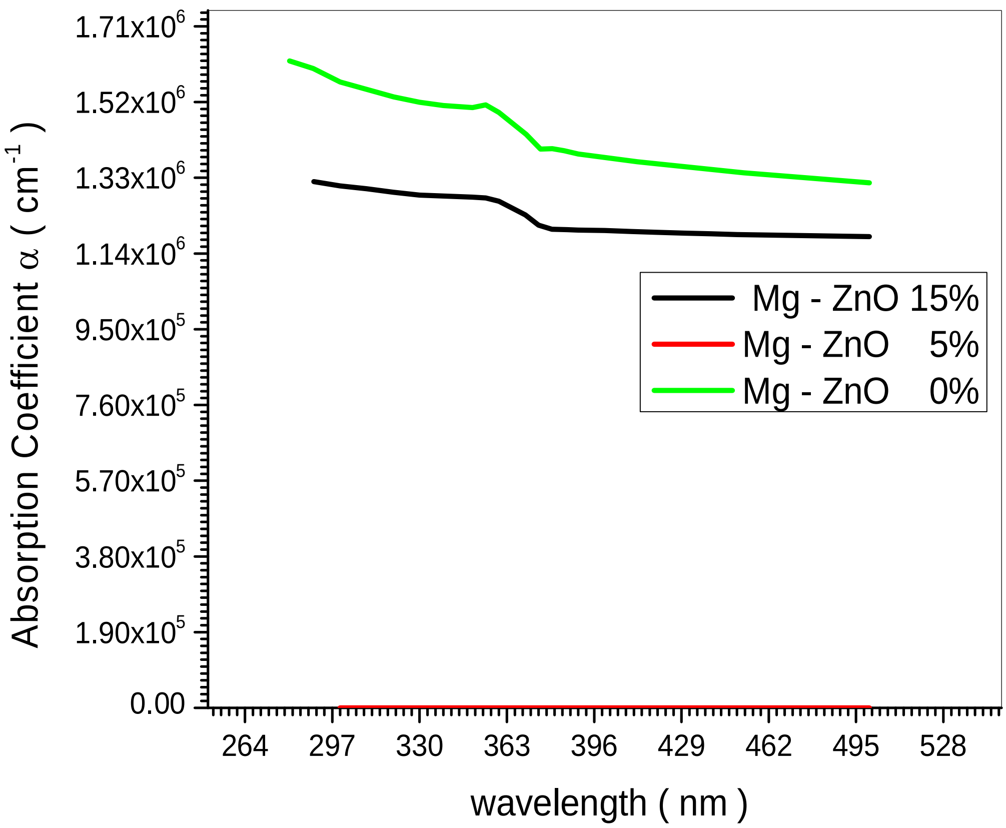



**figure (4-2) Absorption coefficient of $Mg_xZn_{1-x}$ (0.0<x<0.15)**

Fig. (4-2) shows the absorption coefficient α of$Mg_xZn_{1-x}$(0.0<x<0.15) nano particle as a function of the wavelengthfor various Mg contents. The absorption coefficient was calculatedusing the transmittance data, which has been presentedpreviously. Lambert’s Law has been applied to obtain the valueof absorption coefficient at a respective wavelength with the Eq.(4-1) as follows:

$\propto = \frac{1}{t} ln \frac{1}{T}$(4-1) where, $t$ is the thickness and $T$ is the transmittance spectra of samples. The result indicates that all Mg-ZnO nanoparticles samples exhibit high absorptionin the ultra violet (UV) range and low absorption in the visiblerange. The absorption propertiesof MgxZn1-xO $(0.0<x<0.15)$ nano particle in UV range are due to thebehavior of ZnO intrinsic optical bandgap energy. Absorption coefficients in the UVregion significantly increased with Mg progress. The result suggestsimprovement in the optical absorption in the UV regionwith Mg progress, which provides useful information especiallyin the optoelectronic devices and device fabrication.

## 4.3 Band gap energy estimation :

The band gap energy can be determined using the taucrelation , it is convenient way of studying the optical absorption spectrum of material, according to the tauc relation, the absorption coefficient α for direct band gap material is given by

$$(\propto h\gamma)^2 = A(h\gamma - E_g) \qquad 4\text{-}2$$

Where $E_g$ the band gap, A is a constant depending on the electron-holemobility and $E_g$ is the optical bandgap energyconstant ,$h\gamma$ is energy of photon . For determining the band gap energy the tauc plot method used. Figure (4-3) show tauc plot method has the photon enery $(h\gamma)$ on the X axis and aquantity $(\propto h\gamma)$ on the Y axis and extrapolatin the linear portion of the curve to the X axis yields the enery of the materials. the energy gaps of all samples are listed in table (4-1).

Extrapolating the linearpart of the curve that intersects at the x axis will give theoptical band gap energy value. For 0% of $Mg^{+2}$ content whichidentical to ZnO nanoparticle, the optical band gap energy was

3.07ev, With an increment in the Mg content up to 5%, the band gapobtained increased to 3.18 ev, This was followed by 3.2 ev for 15% of $Mg^{+2}$ content, respectively.

An incrementof at least 0.13evin the optical energy band gap was obtainedfrom 0 to 15 at.% of Mg content in Mg-ZnOnano particle. This evidently

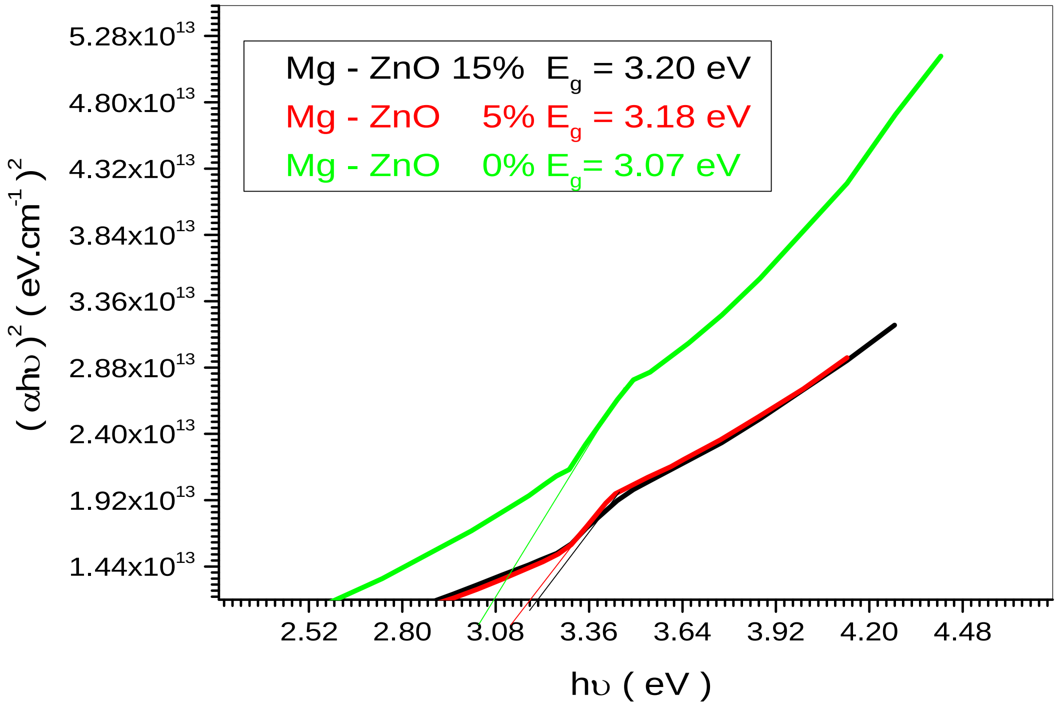



**Figure (4-3) Relation between band gap(eV) vs $(\alpha hc/\lambda)^2$.**

shows that the band gap of ZnOnanoparticle can be altered of the synthesized Mg-ZnOnanoparticle.

**Table** (4.1) show the band gap values of present work **:**

| sample | This work | Theoritcal |
|---|---|---|
| A (0.00) | 3.07 ev | 3.37ev |
| B (0.05) | 3.18ev | |
| C (0.15) | 3.2ev | |

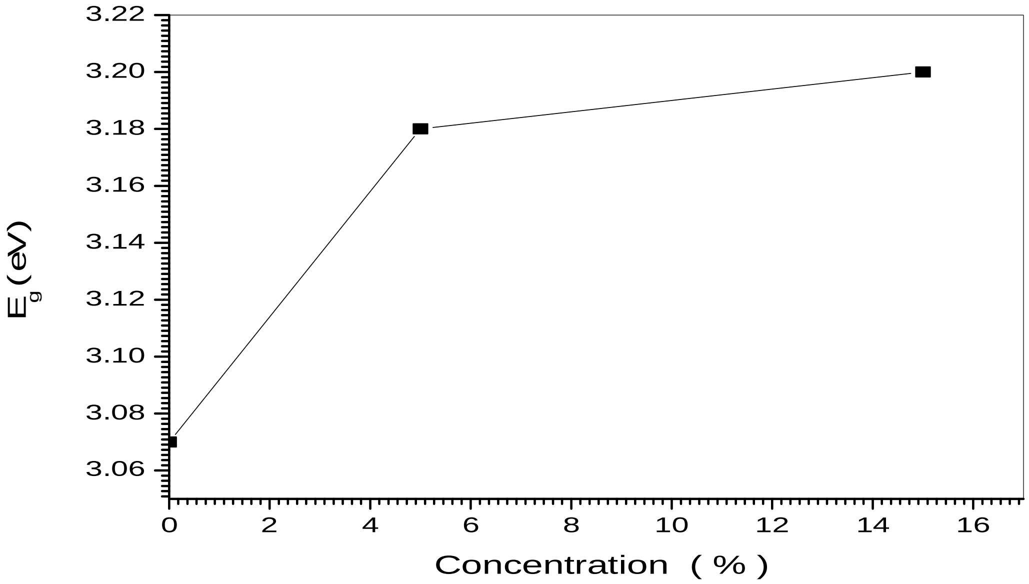



Figure (4.4)shows the increase in the energy gap of Mg- ZnO for differentConcentration of Mg

## 4.4Conclusions:

Nanoparticle samples of Mg-ZnO with different concentration of Mg prepared and optical properties transparency and absorption coefficient has been investigated, and the results indicated that the transparency decrease while absorption coefficient increase with increasing the concentration of Mg, from the results we also concluded that the energy gap increase with increasing the concentration of Mg too.

## 4.5 Recommendations :

- More study and researchesof Mg doped ZnOBecause of its current andpossible applications in several novel devices like UV-gogles.

- Investigation Mg-ZnO properties with other different ratio of magnesium to obtain clear and direct relation between the absorption coefficient and energy gap.

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