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Effect of Nickel Oxide Nano-Particles on Structural and Optical Properties of Casted Polyvinyl alcohol

A research

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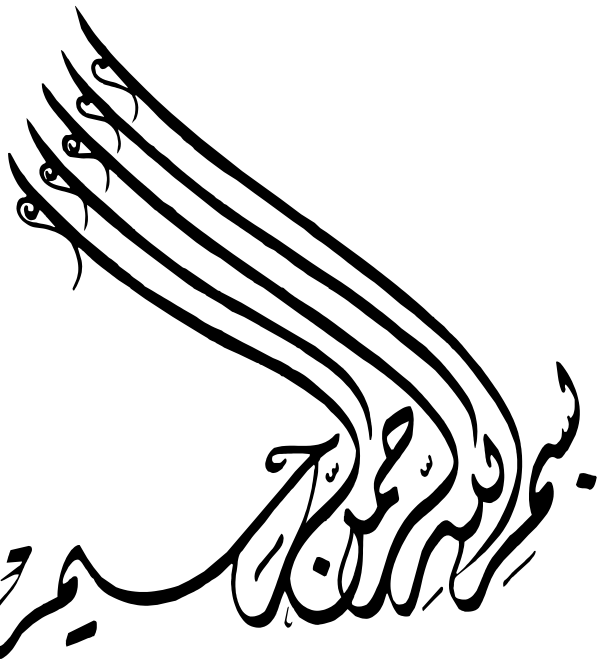

﴿يَرْفَعِ اللَّهُ الَّذِينَ آمَنُوا مِنْكُمْ وَالَّذِينَ أُوتُوا الْعِلْمَ دَرَجَاتٍ وَاللَّهُ بِمَا تَعْمَلُونَ خَبِيرٌ﴾

صدق الله العظيم

(سورة المجادلة: من الآية ١١)

Supervisor Certification

I certify that the preparation of this thesis, entitled **" *Structureal morphological* Effect of Nickel Oxide Nano-Particles on Structural and Optical Properties of Casted Polyvinyl alcohol**

was made under my supervision by ***Hussein Kamel Mohammed Hassan*** at physics department the college of education for pure sciences university of Babylon in partial fulfillment of the requirements .

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In view of the available recommendation, I forward this thesis for debate by the examination committee.

Signature:

Name:

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Date / / 2022.....

Dedication

To mesopotamia(Iraq) with honour and dignity…

To those, Who lost their lives in a war without committing any crime…

To my first and dearest teacher my father…

To my mother whose love is planted in my heart…

To my brothers and sisters…

To my close friends

To my teachers

Who provide me the keys of success

Hussein

Thanks and appreciation

Praise be to God, the first before creation and the last after the annihilation of things, the All-Knowing, Who does not forget those who remember Him, does not diminish from His thanks, does not disappoint those who call upon Him, and does not cut off from His hope.

I would like to thank my supervisor, Professor **Dr. Fouad Shakir Hashim** .

The least that I can offer is a thankful attitude that is unable to fulfill the meaning of this word for suggesting the topic of research and for the commendable efforts he provided me with valuable guidance and sound opinions throughout the research period, which paved the way for me to achieve it. He has my sincere appreciation and respect.

I also extend my sincere thanks and appreciation to the Deanship of the College of Education for Pure Sciences University of Babylon, for giving it the opportunity to complete the study.

I also extend my heartfelt thanks to all my distinguished professors from the Physics Department and all dear colleagues for their support throughout the study period.

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Summary

PVA polymer and its nanocomposites with different weights .% (3, 5, and 7) of NiO NPs were prepared using solution casting method. The results were identified by Fourier transform infrared spectroscopy (FT-IR), optical microscope (OM), and UV-Visible spectroscopy. FT-IR spectra confirmed of the produce the functional groups present in polymer nanocomposite systems. The optical microscope images denote a good homogeneity and fine distribution of NiO NPs.UV-Visible spectroscopy showed that the optimum value of transmittance for polymer film is about 97-98% in the regions Vis and NIR, but it decreases drastically with an increase in the wt.% NiO NPs. Indirect allowed and forbidden transition optical energy gaps were determined from the absorption spectrum, which their values decreased with increasing the ratios of NiO NPs content. The absorbance , absorption coefficientr ,refractive index, extinction coefficient, dielectric constant (real, imaginary) and optical conductivity of PVA are increasing with the increasing of NiO nanoparticles concentrations.

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List of Symbol

Symbol	Physical meaning
PVA	Poly-vinyl alcohol
Nio	Nickel oxide
Erot	rotational energy
Evib	vibration energy
Eele	the electronic energy
Etrans	transitional energy
Tg	Glass transition temperature
Tm	Melting temperature
V.B	Valens band
C.B	Conductive band
E_{act}	Activation energy
$E_g^{opt.}$	Optical power gap
A	The absorbance
I_A	absorbed light intensity
I_o	incident intensity of light
α	Absorption coefficient
λ	wave length

K	extinction coefficient.
Eg	energy gap
N	Refraction index
C	Light speed in vacuum
V	Light speed in matter
R	The reflectivity
T	The transmittance
k	Extinction coefficient
λ	Wavelength of incident ray.
ε	Complex dielectric constant
ε_1	Real part of the dielectric constant
ε_2	Imaginary part of the dielectric constant
R	Optical reflectance
σ_{op}	The optical conductivity
UV	Ultraviolet spectrum
IR	Infrared
ν	the frequency
h	Plank constant
E_{ph}	energy of phonon

Chapter One

Introduction and literature review

1.1 Introduction

Polymer research was born in the great industrial laboratories of the polymer industry. The globe wants to develop and appreciate new types of plastics, rubber, fiber adhesives and coatings. And much later did the science of polymers come to academic life, possibly because of its history, polymer science appears to be more combining chemistry, chemical engineering, materials and other areas as well is interdisciplinary than most disciplines. Chemically, polymers are high molecular weight long-chain molecules, often weighed in the hundreds of thousands, so the term (macromolecules) is primarily used to refer to polymeric materials.

Polymers are often referred to as resins in trade literature, an ancient concept that dates back when the chemical composition of long chains was known. Natural materials, especially cotton, starch, proteins, and wool, were the first polymers used. Synthetic polymers were developed beginning in the early twentieth century. The big possibilities of the new materials were demonstrated by the first polymers of significance, Bakelite and nylon.

The researchers found, however that they did not appreciate many of the interactions between the chemical structures and the corresponding physical properties [1]. The Polymer blends may also be used as high-performance fabrics because the reinforcement properties differ significantly from the matrix properties. The polymer composites have exceptional mechanical strength and rigidity, as well as resistance to corrosion. These properties include improved sensitivity and tolerance to the effects of damping sound and vibration, higher coefficients, a higher application temperature, and more. One of the most popular uses of natural or synthetic polymers is polymer composites.

The polymer-Nano composite mixture is an important aspect of polymer science and engineering because it enables people to produce formulations with previously inaccessible properties by combining normal, uniform, and predictive polymers.

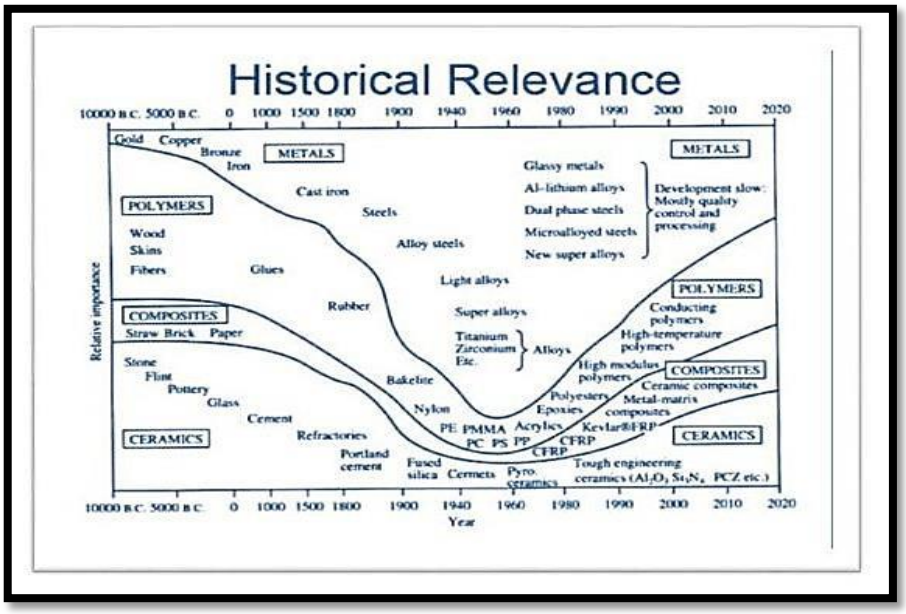


Fig (1-1) The evolution of composite materials from previous centuries until the year 2020 [2]

1.2 Composite Materials

Composite materials are a material system composed of a combination of two or more materials that differ in form or material composition, the properties of a composite are different from those materials [3]. It is also cohesive in structure, the composite is comprised of two major components: the matrix (the basic material) and the additives, the matrix serving to enclose the composite and give it bulk form, it surrounds other constituents and makes them more cohesive to form a "compact system". Additives are constituents added to polymers to provide them with specific properties and improve basic properties, these constituents are added in a granular form or as small particles, Additives can increase the overall conductivity, reduce porosity, improve friction and some magnetic properties …etc [3,4,5] .

1.3 Nanomaterials

Nanomaterials can be defined as a materials with dimensions below 100 nm and they have at least one unique properties that is different from the bulk material and the characteristics can be applied in different fields such as Nano electronics, pharmaceutical and cosmetic. Several methods have been studied in fabricating these nanostructures, which include laser ablation , chemical vapor deposition (CVD) [6], and template-directed growth [7].

in order to integrate one-dimensional nanomaterial into a device, a fabrication method that enables well-ordered nanomaterials with uniform diameter and length is important. Template-directed growth is a nanomaterials fabrication method that uses a template which has Nano pores with uniform diameter and length [8].

using chemical solutions or electro deposition, nanomaterial's are filled into the Nano pores of the templates and, by etching the template, nanowires or nanotubes with similar diameter and length as the template nanopores are obtained. Because the size and shape of the nanomaterial depends on the Nano holes of the template, fabricating a template with uniform pore diameters is very important [9].

Nanomaterials can be classified by different approaches according to the X, Y and Z dimension, according to their shape and according to their composition. A nanomaterial is an object that has at least one dimension in the nanometer scale [10].

Nanomaterials are categorized according to their dimensions into four classes [11].

1. Zero-dimension confinement (quantum dot).
2. One-dimension confinement (quantum wire).
3. Two-dimensions confinement (quantum well).
4. Three-dimensions confinement (bulk).

1.4 Nano composites

Nano composites can be defined as a composite material in which at least one of the phases (mostly the filler) shows dimensions in the nanometer range, as the fillers size reaches the nanometer level, the interactions at the interfaces become considerably large with respect to the size of the inclusion and thus the final properties show significant changes [12].

A nanocomposite, like a traditional composite has two parts, filler and the matrix, a traditional composite typically uses a fiber such as carbon fiber or fiberglass as the filler, in a (NCs) the filler is a nanomaterial.

Some examples of nanomaterial are CNTs, carbon nanofiber, and nanoparticles such as gold, silver, diamond, copper and silicon, of particular interest are CNT (NCs) because of their high strength and stiffness composites they produce at relatively low CNT concentrations [12,13].

1.5 Literature Review

Increased attention has been paid in recent years to researches on polymer composites in general and (NCs) in particular, from the point of view of their potential uses in mechanical, optical, electrical, thermal and ablative applications. A brief summary of recent developments in the above-mentioned fields is given below.

Aman Deep Acharya et al.[14] **,** studied the optical parameters of NiO:PVA composites. Composites contains different concentrations of NiO (0.25 and 0.5 wt%) were successfully fabricated by using solution cast technique. Effect of NiO nanoparticles on various optical properties of PVA such as absorbance, reflectance, extinction coefficient, refractive index, real and imaginary parts of dielectric constant have been studied. The results shows that how a small amount of filler concentration is right enough to produce a drastic change in the polymer matrix.

Karthikeyan et al. [15] , studied the optical, excited-state lifetime, and nonlinear optical (NLO) properties of nickel oxide (NiO)/poly vinylalcohol (PVA) polymer free-standing films for opto-electronics and optical limiting applications. Optical absorption studies of NiO-loaded PVA films show that the exciton peaks are centered at 330 nm. Fluorescence studies reveal that the emission is due to exciton recombination and defects in NiO. Time-resolved fluorescence studies show that the recombination in PVA happens through NiO, where NiO has a faster decay time than the pure PVA. NLO measurements carried out using a 532 nm, 10-ns Nd: YAG laser, show that for a given energy, NiO/PVA shows good optical limiting, and the obtained NLO behavior is due to effective two-photon absorption.

Shaalan et al. [16] , prepared composites of functionalized polyvinyl alcohol by NiO nanoparticles with 1.0–5.0 wt%. Crystal structure analysis were well studied by XRD, Raman and FTIR. The optical properties of the functionalized PVA have been deeply characterized. XRD analysis reveals the polycrystalline feature of pure and functionalized PVA, containing both amorphous and crystalline phases. The structure of the PVA films is influenced by adding the nanoparticles. The dual optical properties exhibit the features of both PVA and dopant materials. Clear change in the optical properties of PVA was observed with various NPs content that has been increased up to 5%. The optical band gap of PVA was changed from 5.4 eV for 0.1% NiO up to higher value at 0.4% NiO. Interesting is the appearance of another indirect band at lower energy. This band gap energy was recorded at 3.8 and 3.36 eV at 0.1% NiO, and 2.85 and 2.3 eV at 0.5% NiO for various phonon energies. The other important optical parameters such as refractive index, dielectric, absorption coefficient, and optical conductivity were evaluated. The observations propose the applicability of the prepared thick film for optoelectronic applications.

Abdullah and Saber [17] **,** studied the optical absorption of polyvinyl alcohol films doped with nickel chloride .They found that the optical energy band gap E_g of the films decreases with increasing $NiCl_2$ contents, while the urbach energy ΔE_t called the width of localized states in the optical band gap decreases from 0.7414 eV to 0.1891 eV .

Sami Chiad et al.[18] , studied the optical properties of silver/ poly (Vinyl Alcohol) (Ag/PVA) films. They found that the optical conductivity increased with the increasing dopant concentration up to 5wt.% of the content. Optical absorption studies in the wavelength range (300–900)nm showed peak in the wavelength region 430 nm for differently doped films, in addition to the peak for undoped PVA. The band edge values shifted to lower energies on doping up to a dopant concentration of 5%wt

Bhat et al. [19] , studied the standard of living has been improved by industrial "revolution" and the demand of new production increases due to population explosion. In the race of industrialization humans are busy discharging harmful gases in atmosphere, dumping unhealthy wastes in soil and discharging of toxic sewage in natural water resources. The present work reports the synthesis of polymer nanocomposite of blend encapsulated with NiO nanoparticles (K1-K5). The polymer nanocomposite films (K1-K5) were characterized by FTIR, XRD, TGA and SEM. The electrostatic interaction between the polymer matrix and encapsulated NiO nanoparticles increases the chemical stability in this order water > NaOH > HCl solution confirmed by contact angle (55° to 99°). The Congo red (CR) dye adsorption values increases in polymer nanocomposite films (K1-K5) were analyzed by an effect by an effect of contact time 45% to 68%, by an effect of CR dye concentration 48% to 70%. But the CR dye adsorption by S3 composite and nanocomposite films (K1-K5) are inversely proportional to the pH scale 4–10. Among four different bacterial strains Bacillus subtilis 25 mm and Staphylococcus aureus 25 mm has shown best antibacterial activity. The result confirms enhancement of antibacterial activity of S3 blend after the doping of NiO

nanoparticles. The present results may be a roadmap to develop some transparent and flexible polymer nanocomposite films for water treatment in textile industries and efficient antibacterial activity.

RaviKumar et al. [20], studied the Nickel oxide (NiO) nanoparticles (NPs) and graphene quantum dots (GQDs) reinforced polyvinyl alcohol (PVA) nanocomposite films were prepared using a solution casting technique. The physicochemical characteristics of PVA/NiO/GQDs (PNG) nanocomposite films were studied using Fourier transform infrared spectroscopy (FTIR), X-ray diffraction (XRD), thermogravimetric analysis (TGA), and field emission scanning electron microscopy (FESEM). The obtained PNG nanocomposite films showed good mechanical flexibility and improved tensile strength. The influence of nanofiller concentrations on PNG nanocomposite film. The obtained results demonstrate an increase in the activation energy (Ea) up to PNG3 upon increasing the GQDs concentration and thereafter, its decreases. The fundamental interactions of the constituents of PNG nanocomposite film were investigated using density functional theory (DFT). This study on electronic structure reveals that the PVA model indirectly interacts with GQDs through the NiO model. This configuration is favoured in terms of interaction energy (−78 kJ/mol) compared to the one in which PVA interacts directly with the GQDs model.

Michalak et al. [21], studied the structural and optical properties of NiO films by using RF magnetron reactive sputtering. Thin films of lithium nickel oxide were deposited by Rf-sputtering from a stoichiometric LiNiO2 target. The XRD tests showed that the diffraction pattern from a 2 μm thick LiNiO film the most intense peaks are due to the pseudo-cubic LixNi1-O phase. The optical measurements shows that the spectral optical constants of LiNiO films as a function of intercalated Lit were reported previously.

1.6 The Aim of the Study

Preparation of a Nano composite (NCs) from polyvinyl alcohol and nickel oxide (PVA-NiO) by the method of pouring the solution and studying its structural and optical properties

Chapter Tow
Theoretical Back Ground

2.1 Introduction

This chapter includes a general description of the theoretical part of this study, physical concepts, scientific explanations, relationships, and laws used to interpret the study results.

2.2 Polymer Structure

Polymer science was arise the great industrial laboratories of the world of the need to make and understand new kinds of plastics, rubber, adhesives, fibers, and coatings. polymer science come to academic life perhaps because of its origins, polymer science tends to be more interdisciplinary than most sciences, combining chemistry, chemical engineering, materials, and other fields [24].

It should be noted that the term monomer or monomer unit is often used to mean either the chemical repeat unit or the small molecule that polymerises to give the polymer. These are not always the same in atomic composition, as will be clear from what follows, and the chemical bonding must of course be different. The simplest polymers are chain-like molecules of the type:

−A-A-A-A-A-A-A-A-A-A-A-A-A−

Where A is a small group of covalently bonded atoms and the groups are covalently linked. The simplest useful polymer is polyethylene [25].

− CH_2 − CH_2 − CH_2 − CH_2 − CH_2 − CH_2 − CH_2− CH_2 − A polymer is a large molecule built up from numerous smaller molecules. These large molecules may be linear, slightly branched, or highly interconnected. In the latter case, the structure develops into a large three-dimensional network. The small molecules used as the basic building blocks for these large molecules are known as monomers. For example, the commercially important material poly (vinyl chloride) is made from the monomer vinyl chloride. The repeat unit in the polymer usually corresponds to the monomer from which the polymer was made.

There are exceptions to this, though. Poly(vinyl alcohol) is formally considered to be made up of vinyl alcohol (CH_2CHOH) repeat units but there is, in fact, no such monomer as vinyl alcohol [26].

2.3 Classification of Polymers

2.3.1 Thermal classification of polymers:

Polymers are classified according to the effect of temperature into:

a. Thermoplastic polymers:

The properties of these polymers are changed by the effect of temperature. When the temperature increases, This material becomes elastic and sticky.

By lowering temperature, these polymers return to their original solid state because the molecules in a thermoplastic polymer are connected by relatively weak intermolecular forces (Vander Vales forces), When heated, these molecules can slide over each other as in polystyrene, polyethylene, polypropylene, polyvinyl chloride and Polyvinyl alcohol . [27].

b. Thermoset Polymers:

These polymers are chemically changed when heated. Thermosets are usually three-dimensional networked polymers in which there is a high degree of cross-linking between polymer chains. After being heated, these polymers become insoluble, non-conductive of heat and electricity and hard because molecules of these polymers are connected by strong covalent chemical. Phenol formaldehyde resin and urea-formaldehyde resin are examples of this type of polymers [28].

2.3.2 Chemical classification of polymers

Polymers are classified depending on the structural composition in to:

a. Linear polymers:

The essential structural unit for these polymers is one molecular series of certain length connected with each other in a linear shape, it does not contain the branch except the totals twisted which is part of monomer[26] as in figure.(2-1,a).

b. Branched polymers:

Here the long chain is branching and it is characterized by this type of installation that the branches as a Ladder or a Comb or as a Crusader , The branches have different lengths[25] as in figure. (2-1,b).

c. Cross linked polymers:

In this type, the chemical bonds are interwoven with each other in a complex way. The format string consists of three dimensional polymerhains linked together by more than one site, or when use monomers containing effective totals rather than being included in two effective totals [24] as in the figure. (2-1, c).

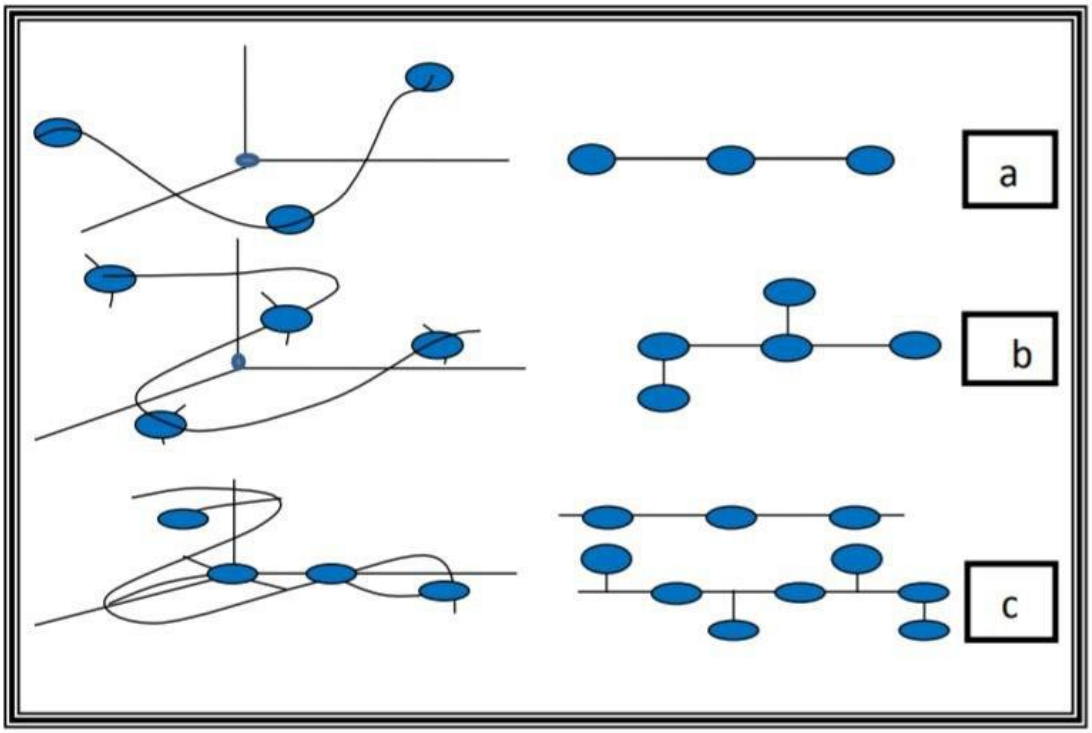


Fig (2-1): The types of polymeric chains [29]

a-Linear b- Branched c- Cross linked

2.3.3 Polymers dependent on homogeneity

Polymers are classified depending on the homogeneity of repeating units into:

a. Homo polymers:

Where the building blocks of a polymer are of one type in poly therphethals ethylene [25].

b. Copolymers:

Where the building blocks of a polymer are more than one type, as in the polymer styrene - butadiene [26].

c. Composite Polymers:

It is the process of adding some material to homogeneous polymers in order to change in some of its characteristics and the entering of new
recipes on it [24].

2.3.4 Polymers dependent on the chains lengths and molecular weights

a. Mono disperses polymers:

All particles in this case are of equal size and have the same weight, this type of polymers is not common [29].

b. Poly disperses polymers:

Polymers resulting from polymerization consist of a wide range of molecular weights, i.e., different chains in length, where not all chains grow during the polymerization process to the length itself. This means that he existence of a diverse distribution of the lengths of the chains and thus there is a multiplicity of molecular weights [30].

2.4 Polymers Sources

Polymers are two main sources:

a. Natural polymers:

It is compounds come from plant or animal such timber, cotton , natural rubber, wool and silk. The natural food that is the natural polymers is starch, protein and cellulose [31].

b. Synthetic polymers:

A polymer which is prepared from simple chemical compounds and represent the most industrial important polymers, including plastics, synthetic leather, nylon fabrics and some other dyes [32].

2.5 Poly(vinyl alcohol) (PVA)

Polymers have drawn considerable interest in device fabrication because of their extraordinary inherent properties[33,34], like easy processability, flexibility, high mechanical strength, etc. It is well documented that the electrical and optical properties of polymers can be improved to the desired limit through suitable doping [35]. Poly (vinyl alcohol) is a synthetic polymer and is an odorless, translucent, tasteless, white, or cream-colored granular powder [36]. It is one of the earliest and best-known polymers, it uses in a variety of applications and currently is extensively used in semiconductors applications. It has the formula $(C_2H_4O)_n$, as shown in figure (2.1) [37] and table(2.1) [42]. The advantage of poly (vinyl alcohol) that can blend into the water, which is resistant to do solvents, oils and has the exceptional [38]. Poly (vinyl alcohol) is a Semi-crystalline and has a very high transmission for visible light. Polymeric composites of PVA are known as very important in various technical applications [39]. It is produced commercially by the hydrolysis of poly (vinyl acetate).

Many researchers have been investigated the PVA to use as fillers or cross-linked products, also it has been widely applied to manufactured nontoxic, harmless and living tissues, etc. as a thermoplastic polymer[40,41]. Moreover, It is very

advantageous to form the film that makes it a strong candidate to use for blending natural polymers and other polymers [42,43] . PVA is commonly used to coat the paper as well as in sizing the textile because of its biodegradable futures [44]. PVA is employed in several applications because it is an ability incompatible structure and hydrophilic properties that assist to improve the mechanical properties of films [45,46]. Additionally, nanoparticles could physically entangle or chemically bound with PVA [40]. It's widely used in making paper and textile industries in the manufacture of membranes resistance to oxygen in the coating photographic film [38].

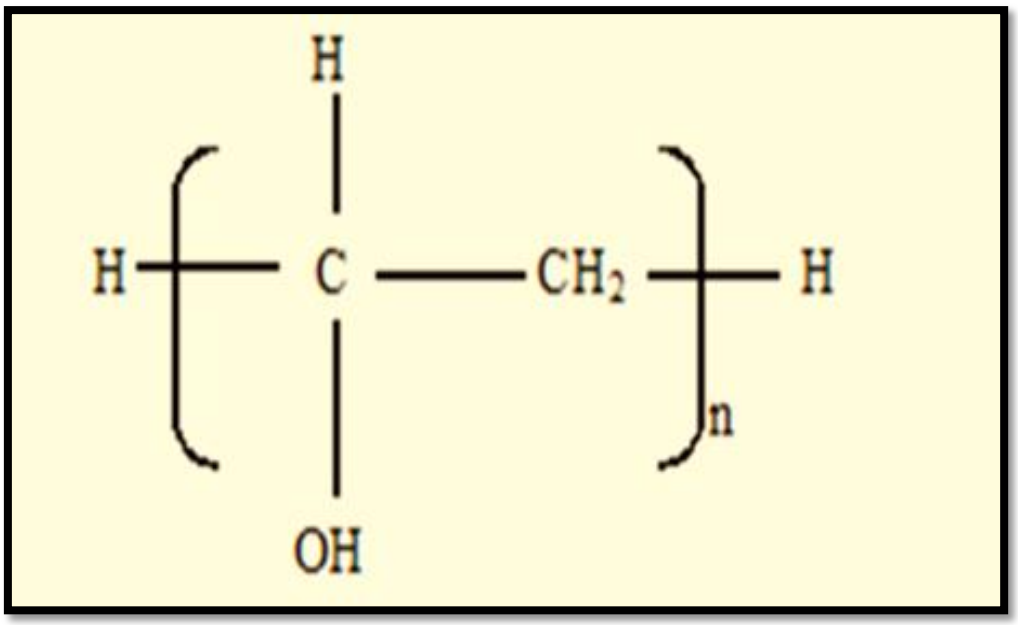


Fig (2.2): The Chemical Structure of PVA [37]**.**

Table(2.1): Physical and Chemical Properties of Poly(vinyl Alcohol) (PVA)[42]**.**

Property	Description
Appearance	White to an ivory white granular powder
Molecular formula	$(C_2H_4O)_n$
Solution PH	5- 6.5
Density g/cm^3	1.3 g/cm^3
Refractive index	1.55
Glass transition temperature T_g ºC	85 ºC
Melting temperature T_m ºC	230 ºC

2.6 Properties and Application of NiO

Metal oxide semiconductors have attracted a wide interest owing to their unique properties and massive potential applications in different fabrication. Nickel (II)oxide is the chemical compound with the formula NiO. It is a transition metal oxide having a wide band gap in the range from 3.6 to 4.0 eV [46]. NiO is an important antiferromagnetic p-type of semiconductor and is a promising for many applications such as lithium ion batteries , solar cells, antiferromagnetic layer, electrochemical capacitors, chemical sensors , and electrochromic coatings [47]. Stoichiometric NiO at room temperature is an insulator with a resistivity of 10^{13} Ω cm. Table (1.1) shows the physical and chemical properties of the NiO structures. NiO adopts the NaCl structure as shown in figure (2.3) [48] and table(2.2)[60], with octahedral Ni(II) and O^{-2} sites. The conceptually simple structure is commonly known as the rock salt structure .

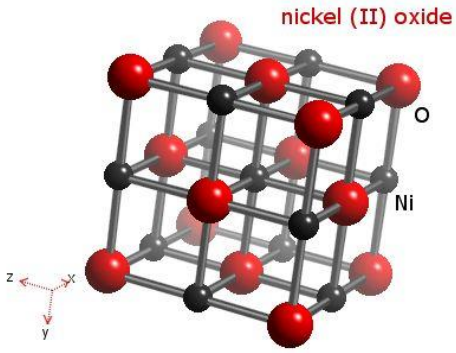


Fig. (2.3): Lattice structure of NiO [48].

Table (2.2): Physical and chemical properties of NiO [60]

Properties	Specification
Molecular formula	NiO
Crystal system	Cubic
Crystal structure	Rock salt-type structure
Color	greenish black
Molar mass (g/mol)	74.693
Density (g/cm^3)	6.67
Melting point (°C)	1955
Refractive index (n_D)	2.1818
Energy gap (eV)	3.6 -4.0
Resistivity (Ω cm)	10^{13}
a (Å), b (Å), c (Å)	4.178(1), 4.178(1), 4.178(1)
α (deg), β (deg), γ (deg)	90،90 ،90

2.7 Optical Properties

The study of the optical properties of polymers increases our knowledge of the type of polymer internal structure; nature of the bonds and expands the potential scope of polymer application, Knowing the spectrums of absorption and

transmittance a polymer assist in identifying many optical properties in different ranges of wavelengths. Conducting examination at the ultraviolet spectrum range enables us to know the type of the bonds, orbital and energy beams. The study at the visible spectrum range provides sufficient information about the behavior of a matter to solar applications. The study at the infrared range is very important in knowing the general structure of a polymer and the elements consisting its chemical structure [49]. Knowing the spectrum of absorption and transmittance of a polymer assist in identifying many optical properties in different ranges of wavelengths. Conducting examination at the ultraviolet spectrum range enables us to know the type of the bonds, orbital and energy beams. Optical properties are commonly characterized using spectroscopic techniques including UV-visible and photoluminescence spectroscopy, which both yield information about the electronic structure of nanoparticles [50].

2.7.1 Light absorbance and electronics transitions

The total molecular energy has divided into the electronic energy (E_{ele}), vibration energy (E_{vib}), rotational energy (E_{rot}) and transitional energy (E_{trans}). The absorbance of electromagnetic wave results in a change in the total energy of the molecule due to the change in the different energies [51].

$$\Delta E_{total} = \Delta E_{vib} + \Delta E_{rot} + \Delta E_{ele} + \Delta E_{trans} \quad \text{.....(2-1)}$$

It has been noted that the visible and ultraviolet spectrums are the spectrum of electronic absorbance; the remaining is the spectrum of other absorbance. The E_{ele} is the clearest in the absorbance spectrum. The reaction of the photon with the molecule makes the electrical field of the photon works in a manner that agitates the electronic structure of the molecule to the point that makes the photon disappear and its energy transferred to the molecule whose state has been changed to an excited state [52]. figure (2.4) shows the energy regions and molecular energies.

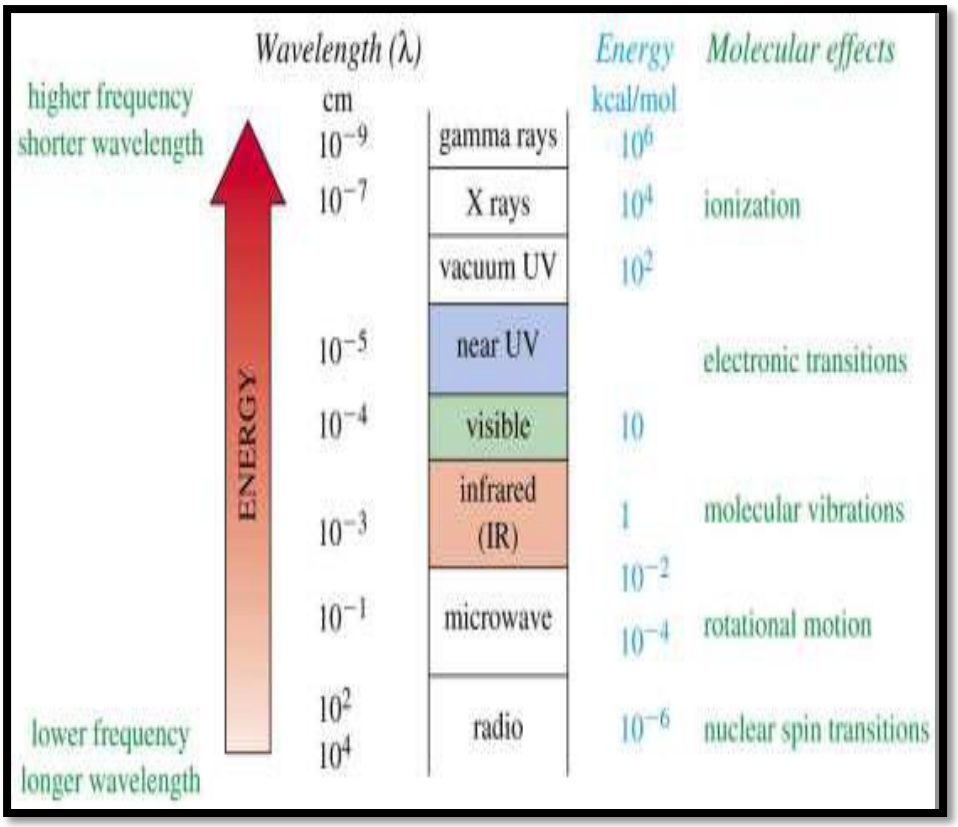


Fig (2.4): The electromagnetic spectrum region [53].

2.7.2. Optical absorbance (A)

Absorbance can be defined as the ratio between absorbed light intensity (I_A) by material and the incident intensity of light (I_o) [54].

$$A=I_A/I_0 \quad \text{……..……(2-2)}$$

2.7. 3. Optical transmittance (T)

It is the ratio between the intensity of the beam from the film I_T to the intensity of the beam incident on the film thin I_O and expressed by the relationship [55].

$$T=I_T/I_o \quad \text{…….……..……..(2-3)}$$

2.7. 4. Optical reflectance (R)

The absorbance (A) and transmittance (T) can also be calculated from the following equation [56]:

$$R + A + T = 1 \quad \text{……..…….(2-4)}$$

Where: R: reflectance, T: transmittance, and A: absorbance.

When the fall of the beam of monochromatic light perpendicular to the section of the surface of the samples the part of the beam will reflect and implement the remaining part. This force could face the process of absorption also in order to keep the algebraic sum of these parts equal to the value one.

2.7.5. Optical constants

There are many ways to find the optical constants of absorption coefficient, refractive index, extinction coefficient, the complex of dielectric constant (real and imaginary) and optical energy gap:

1. Absorption Coefficient (α)

The optical absorbance coefficient (α) of the film is given by the equation [51]:

$$\boldsymbol{\alpha} = 2.303A/d \quad \text{.....(2-5)}$$

Where (d) represent a thickness of sample.

2. Refractive Index (n)

It is the ratio of light speed in vacuum to its speed in a medium. This index shows how far a matter is affected by the electromagnetic waves. The refraction index consists of two parts: real and imaginary. It can be expressed by the following equation [56];

$$n = c/v \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \text{(2-6)}$$

where (n) is the refraction index, (c) is the light speed in vacuum and (v) is the light speed in matter. Reflectance (R) can also be defined as the ration of the reflected ray relation at the borderline between two mediums to the incident ray. The relation between reflectivity and refractive index is shown in the following equation;

$$R = (n-1)^2 + k^2 /(n+1)^2 + k^2 \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \text{(2-7)}$$

where (k) is the extinction coefficient.

The rate of absorption of light is directly proportional to the intensity of the incident light at a specific wavelength, and this physical phenomenon is common and lead to the decay of the light intensity exponential as it passes.

Refractive index can be expressed by the following equation [57];

$$n = [4R/(R-1)^2 - k_o^2]^{1/2} + (R+1)/(R-1) \quad \ldots\ldots\ldots\ldots\ldots\ldots\text{(2-8)}$$

Where k is the extinction coefficient. The reflectance of thin films was measured directly by using the Specular Reflectance Attachment (with 5^o incident angle) of the UV-Vis-NIR double beam spectrophotometer (Shimadzu, UV-1800). The technique of specular reflectance is often applied to the examination of semiconductors, optical materials, multiple layers, etc. The 5^o incident angle minimizes the influence of polarized light. Thus, no polarizer is needed to perform the reflectance measurements.

3. Extinction Coefficient (k)

The electrical coefficient the amount of photons absorbed by the membrane, that is, the energy absorbed by the electrons of the material, and expresses the following relationship [53]:

$$k = \alpha\lambda/4\pi \quad \ldots\ldots(2\text{-}9)$$

Where (λ) is the wavelength of the incident ray and (α) absorption coefficient.

4. Complex Dielectric Constant

The matter of ability of polarization is represented the dielectric constant. The matter is reflected to various frequencies in a complex manner. at optical frequencies, it is characterized by the waves of the light, where the electronic polarity considered as dominating above all other remaining polarization types. and this polarization is called dielectric constant known as the following relationship [58].

$$\varepsilon = \varepsilon_r - i\varepsilon_i \quad \ldots\ldots(2\text{-}10)$$

Where ε_r the real part of the dielectric constant, ε_i the imaginary part of the dielectric constant.

$$\varepsilon = N^2 \quad \ldots\ldots(2.11)$$

$$(n - ik)^2 = \varepsilon_r - i\varepsilon_i \quad \ldots\ldots(2.12)$$

From equation (2.10) real and imaginary complex dielectric coefficient can be written as follows [58]:

$$\varepsilon_r = (n^2 - k^2) \quad \ldots\ldots(2.13)$$

$$\varepsilon_i = (2nk) \quad \ldots\ldots(2.14)$$

The optical conductivity (σ_{op}) depends directly on the refractive index (n) and absorption coefficient (α) by the following relation [59]:

$$\sigma_{op} = \alpha nc/4\pi \quad \ldots\ldots(2.15)$$

2.7.6 Fundamental absorption edge

The fundamental absorption edge can be defined as the rapid increasing in absorbance when absorbed energy radiation is almost equal to the band energy gap; therefore, the fundamental absorption edge represents the less difference in the energy between up point in valance band to bottom point in conduction band [60].

2.7.6.1 Absorption regions

Absorption regions can be classified to three regions [61]:

A) High absorption region

This region is shown in figure (2.4). In part (A), the magnitude of absorption coefficient (α) is larger or equal to (10^4 cm^{-1}). From this region the magnitude of forbidden optical energy gap (Eg^{opt}) can be introduced.

B) Exponential region

This region is shown as in figure (2.5). In part (B) the value of absorption coefficient (α) is equal to ($1\ cm^{-1} < \alpha < 10^4\ cm^{-1}$). It refers to transition between the extended levels from the Valens band (V.B.) to the local level in the conductive band (C.B.) and vice versa, transited from local levels in (V.B.) to the extended levels in the bottom of conductive band (C.B.).

C) Low absorption region

The absorption coefficient (α) in this region is very small, it is about ($\alpha<1cm^{-1}$). The transition happens in this region because of state density inside space motion resulted from faults structural [63], as in figure (2.4)

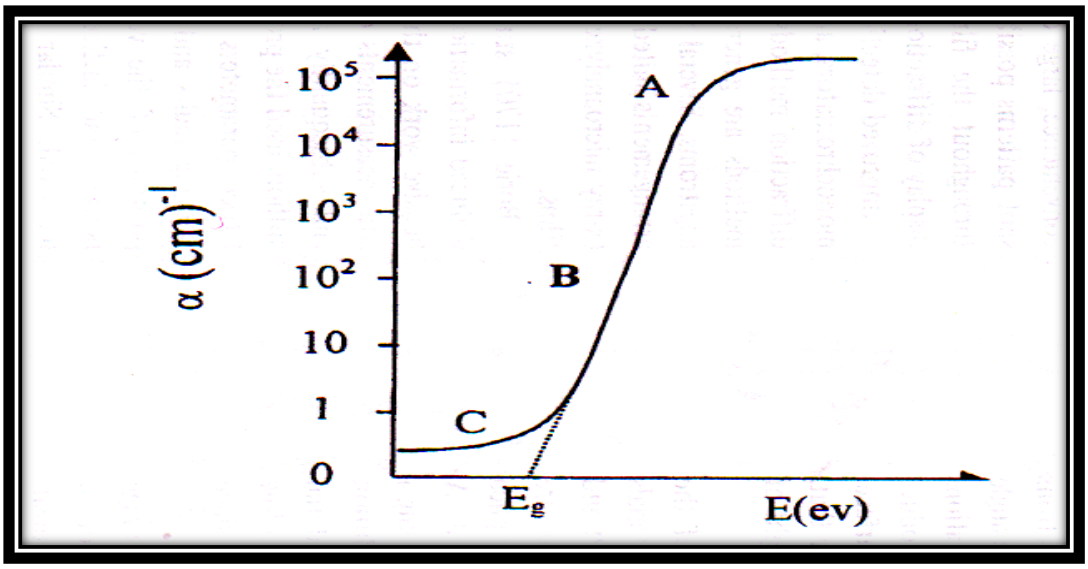


Fig (2.5):The variation of absorption edge with absorption regions [62].

2.8 The Electronic Transitions

Electronic transitions are divided into two types:

2.8.1 Direct transitions

Direct transitions occur when conduction band(C.B) and valance band at the same point in the space .This means that they have the same value of wave vector ($\Delta K=0$). In this case the absorption will appear at ($Eg=hv$). This type occurs without a noticeable change in energy and momentum. There are two types of direct;

2.8.2 Allowed direct transition

Figure (2.5.a) shows that this transition happens from top points in the valence band (V.B) and the bottom point in the conduction band (C.B). The empirical relationship for this type of transition is given by the equation [59]:

$$\alpha h\nu \approx B[h\nu - Eg]^{1/2} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \text{(2-16)}$$

Where (α) is the absorption coefficient, (h) Plank constant (6.625×10^{-34} $J.s$), (ν) is the frequency in (Hz), (E_g) energy gap.

2.8.2 Forbidden direct transitions

Figure (2.5.b) Shows that this transition happens from near the top points of valence band (V.B) and the bottom points of conduction band (C.B). The empirical relationship which corresponds to this transition is given by the equation [64]:

$$\alpha h\nu \approx B\,[h\nu - Eg]^{3/2} \qquad \text{.....(2-17)}$$

2.8.3 Indirect transition

This transition happens when the bottom of conduction band (C.B) is not over the top of valence band (V.B), in curve (E-K) Fig (2-5). The electron transits from V.B are not perpendicularly, where the value of the wave vector of electron before and after transition is not equal ($\Delta k \neq 0$). This transition type happens with the help of a like particle called "Phonon". There are two types of indirect transitions, this type of transitions occur by help phonon to conservation of movement resulted from variation in wave vector for the electron.

$$h\nu = E_g \pm E_p \qquad \text{.....(2-18)}$$

where E_p is the energy of absorbed or emitted phonon.

2.8.4 Allowed indirect transitions

Figure (2.5.c), in the case of moving from the highest point of the valence band to the lowest point of the bottom of the conduction band, which are found in the difference region of K-space [65].

$$\alpha h\nu \approx B\,[h\nu - Eg]^2 + EPh_0 \qquad \text{.....(2-19)}$$

2.8.5 Forbidden indirect transitions

These transitions happen between near points in the top of (V.B.) and near points in the bottom of (C.B.) [66,67], as shown in fig.(2.5-d). The absorption coefficient for transition with a phonon absorption is given by :

$$\alpha h\nu = B(h\nu - E_g^{opt} \pm E_{pn})^r \qquad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(2\text{-}20)$$

Where: E_{ph}.: energy of phonon, is (-) when phonon absorption, and (+) when phonon emission.

(r = 2) for the allowed indirect transition.

(r = 3) for the forbidden indirect transition.

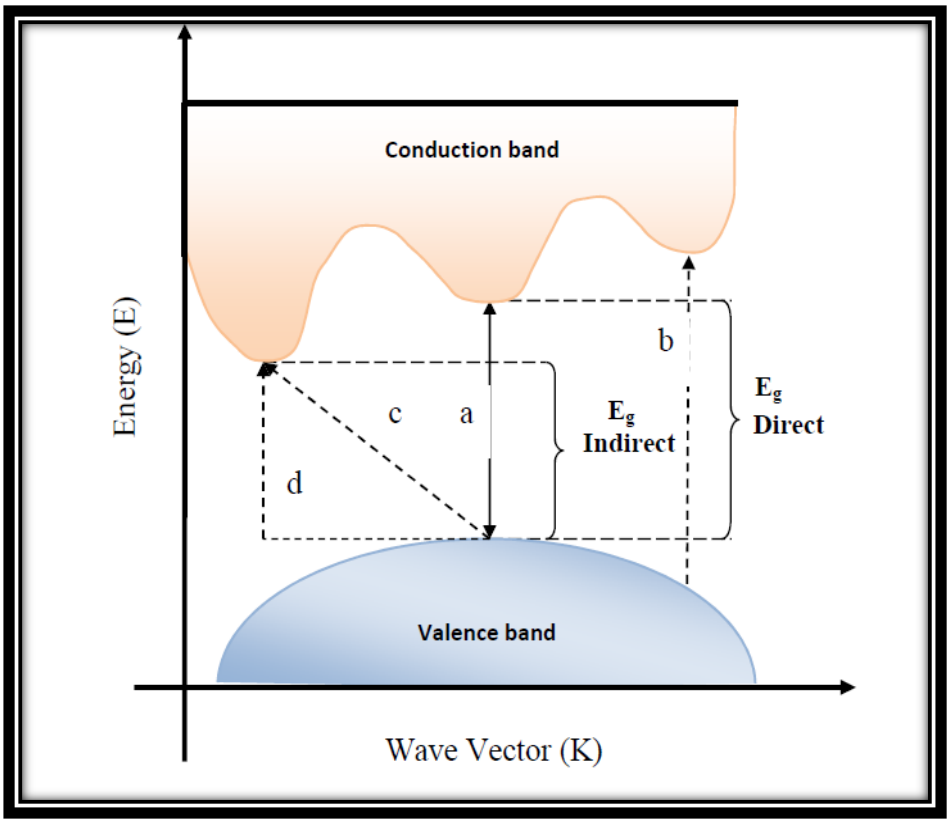


Fig. (2.6) The types of transition [65].

(a) allowed direct, (b) forbidden direct, (c) allowed indirect, and (d) forbidden indirect.

Chapter Three
Experimental Work

3.1 Introduction

This chapter includes an explanation of the stage of preparing the nanocomposites with a general description of the materials used in preparing the models (PVA-Nio) and the stages of conducting the tests in order to know the effect of adding nano-nickel oxide on the structural and optical properties, with a general description of the devices used in the preparation and examination stages.

3.2 The materials used in the study

3.2.1 Base material

In this research, one type of polymer was used .

3.2.1.1 Polyvinyl alcohol

Polyvinyl alcohol used as granular form has a melting point of 230 ℃ and was prepared by (Panreac/Spain) company, with a high purity of 99% and a molecular weight (160000 g. mol^{-1}), Distilled water is considered a good solvent for this substance.

Fig (3-1): Poly vinyl alcohol material.

3.2.2 Additive

In this research, one type of nanomaterials was used

3.2.2.1 Nano nickel oxide

Nano nickel oxide is a black powder with nano granular size

3.3 Sample preparation

3.3.1 First sample

The first sample, the polymeric material, was first prepared by dissolving (1 g) of polyvinyl alcohol in a volume (50 ml) of distilled water inside a glass beaker with a capacity of (100 ml) using a (magnetic stirrer) In a mixing process to obtain a more homogeneous solution, at a temperature of 85 ℃ and a time (45minutes), and then this model was poured with plastic bases (petridish).

It is placed on a horizontal surface after balancing it with an accurate balance and then left to dry for 7 days at room temperature.

3.3.2 Second sample

0.97 g of PVA was dissolved in a volume of 50 ml of distilled water in a glass beaker with a capacity of 100 ml, at a temperature of 85 ℃ and with a time of 45 minutes.

Then 0.03 g of nano-nickel oxide was added, and then it was left for 30 minutes and after it was poured with a plastic base (petridish) placed on a horizontal surface weighed by a fine scale, and then left to dry for 7 days.

3.3.3 Third sample

0.95 g of PVA was dissolved in a volume of 50 ml of distilled water in a glass beaker with a capacity of 100 ml, at a temperature of 85 ℃ and with a time of 45 minutes.

Then 0.05 g of nano-nickel oxide was added, and then it was left for 30 minutes and after it was poured with a plastic base (petridish) placed on a horizontal surface weighed by a fine scale, and then left to dry for 7 days.

3.3.4 Fourth sample

0.93 g of PVA was dissolved in a volume of 50 ml of distilled water in a glass beaker with a capacity of 100 ml, at a temperature of 85 ℃ and with a time of 45 minutes.

Then 0.07 g of nano-nickel oxide was added, and then it was left for 30 minutes and after it was poured with a plastic base (petridish) placed on a horizontal surface weighed by a fine scale, and then left to dry for 7 days.

Fig (3.2): Magnetic stirrer

Table (3.1): Weight percentages for nanocomposites.

PVA %	NiO %	Wt.
1	0	1g
0.97	0.03	
0.95	0.05	
0.93	0.07	

3.4 Laboratory equipment and tests

3.4.1 Optical Microscope

Optical Microscope is a type of microscope that uses visible light and a system of lenses to magnify images of small samples. Optical microscopes are the oldest design of microscope and were possibly designed in their present compound form in the 17th century. Basic optical microscopes can be very simple, although there are many complex designs that aim to improve resolution and sample contrast. Historically, optical microscopes were easy to develop and are popular because they use visible light, so samples may be directly observed by the eye [66].

In order to determine the homogeneity of (NCs) (PVA-Nio) and the amount of diffusion of nickel oxide nanoparticles (NiO), a test of samples with different concentrations of the additive was carried out using a light microscope that was prepared by Olympus (Nikon-73346), as shown in Figure (3-4), which contains an automatic controlled light intensity camera. Under the power of magnification (100 x), which is located at the University of Babylon / College of Education for Pure Sciences - Department of Physics.

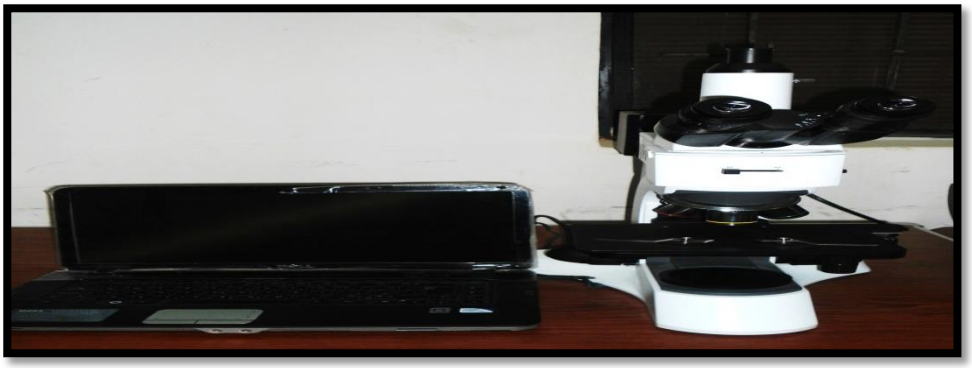


Fig. (3.3) Image of the optical microscope.

3.4.2 Spectrophotometer

A spectroscope that is used to me asure the properties of light in a specific field of the electromagnetic spectrum for the study and identification of materials in spectroscopy. Through the device, it is possible to determine the emission and absorption spectrum, know the wavelength and the optical intensity of the spectral lines [54].

The absorbance spectrum of the nanocomposite (PVA-Nio) was recorded using a device (1800-Spectrophotometer model UV-UV) manufactured by (Shimadzo) company at room temperature and for a range of wavelengths (190-1100) nm as shown in the figure (5-3), and from the results of the absorption spectrum, the transmittance, energy gap, absorption coefficient and the rest of the optical constants were calculated. The measurements were made at (College of Education for Pure Sciences - University of Babylon).

Fig. (3.4) Photograph of the UV Spectrophotometer.

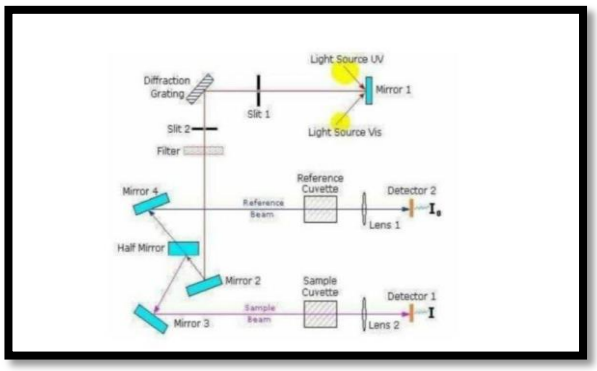


Fig. (3.5) Diagram showing the components of the optical spectrometer

3.4.3 Fourier transform infrared Spectrometer

Fourier-transform infrared spectroscope (FTIR) is a technique used to obtain an infrared spectrum of absorption or emission of a solid, liquid or gas. An FTIR spectrometer simultaneously collects high-spectral-resolution data over a wide spectral range (Fig.2.2). This confers a significant advantage over a dispersive spectrometer, which measures intensity over a narrow range of wavelengths at a time. The term Fourier-transform infrared spectroscopy originates from the fact that a Fourier transform (a mathematical process) is required to convert the raw data into the actual spectrum. The goal of any absorption spectroscopy (FTIR, ultraviolet-visible "UV-Vis" spectroscopy, etc.) is to measure how much light a sample absorbs at each wavelength. [68].

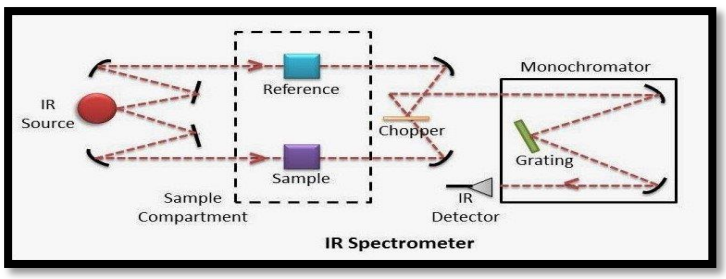


Fig. (3.6): Fourier Transfer Infrared Spectroscopy (FTIR) [69].

It is a device manufactured by the German company (Bruker company) of the type (Vertex-70) shown in Figure (6-3). The FT-IR spectrometer is characterized by the fact that it analyzes small samples with a faster and more accurate degree than the normal device, as this device works for a range of settings The wavelength ranges between (500-4000) cm-1 and the main purpose of using it is to know the occurrence of a chemical reaction for the nanocomposite, that is, it is just a good physical mixture.

Fig. (3.7) Image of the FT-IR device.

Chapter Four

Chapter Four: Results and Discussions

4.1 Introduction

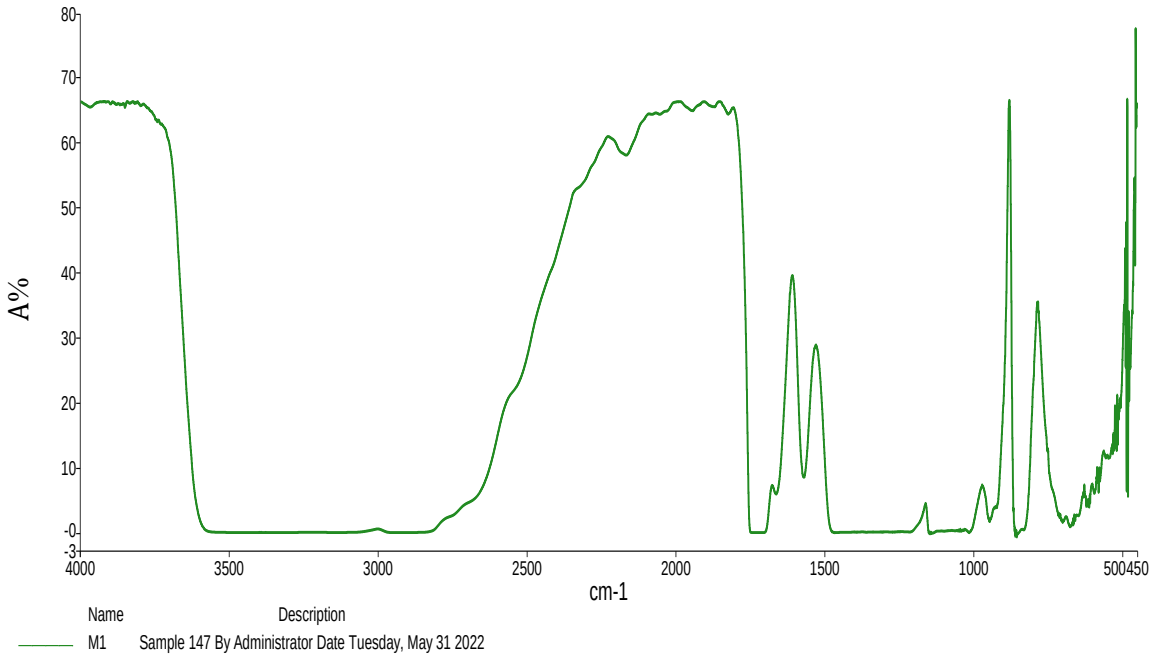
This chapter comprehensive evaluation the results obtained for the effect different ratios of NiO NPs on the structural, and optical properties of PVA polymer and analysis of the results based on changes.

4.2 Fourier transform infrared radiation (FT-IR) of the casting samples

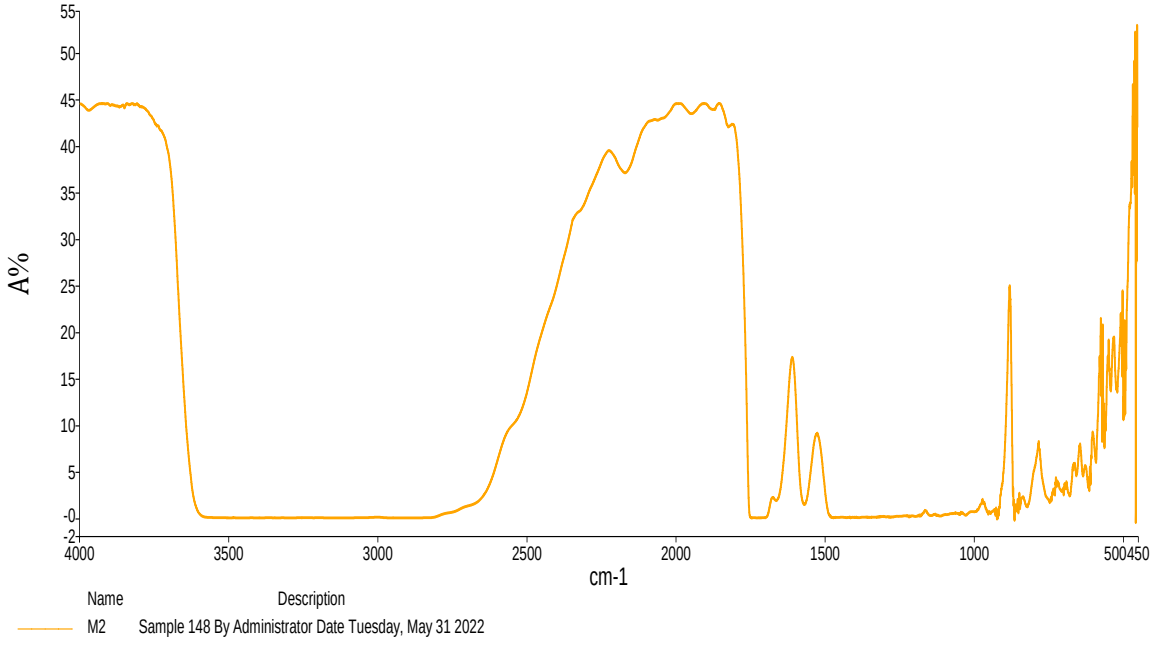
FT-IR spectroscopy is one of the tools to provide useful information regarding the interactions between their functional groups. IR analysis is carried out on a FT-IR transmission profile spectrum to characterize the interface of PVA polymer and its NC films with different wt.% of NiO NPs under the investigated at RT in wavenumber (500-4000) cm^{-1} ranges.

Figure (4.1) illustrates the FTIR spectra of PVA and its NCs with different wt.% (3, 5, and 7) of NiO NPs. The function groups of PVA appeared at 3310.88 cm^{-1}, 2903.50 cm^{-1}, 2167.08 , 1724.21 , 1047.38 cm^{-1} corresponding to broad band to the hydroxyl groups' stretching vibrations O–H, Methyl C-H_3 asymmetric stretching band, medial alkyne (disubstituted) C≡C group, C=O stretching of the ester group carbonyl groups, C-O stretching vibration, respectively. The bands showed at 840.00 and 700.00_cm^{-1} are allocated to peroxide C–O–O– stretching, and C-H stretching, respectively. For ease of follow-up see Table 4.1.

The transmittance decreases with the increasing ratios of NiO NPs that assigned to increase the density of NPs. From this analysis, it is understood that there are no new peaks of absorption, therefore no interactions between polymer matrix and NPs[68].


A%
cm-1
4000
3500
3000
2500
2000
1500
1000
500450
Name
Description
M1
Sample 147 By Administrator Date Tuesday, May 31 2022

a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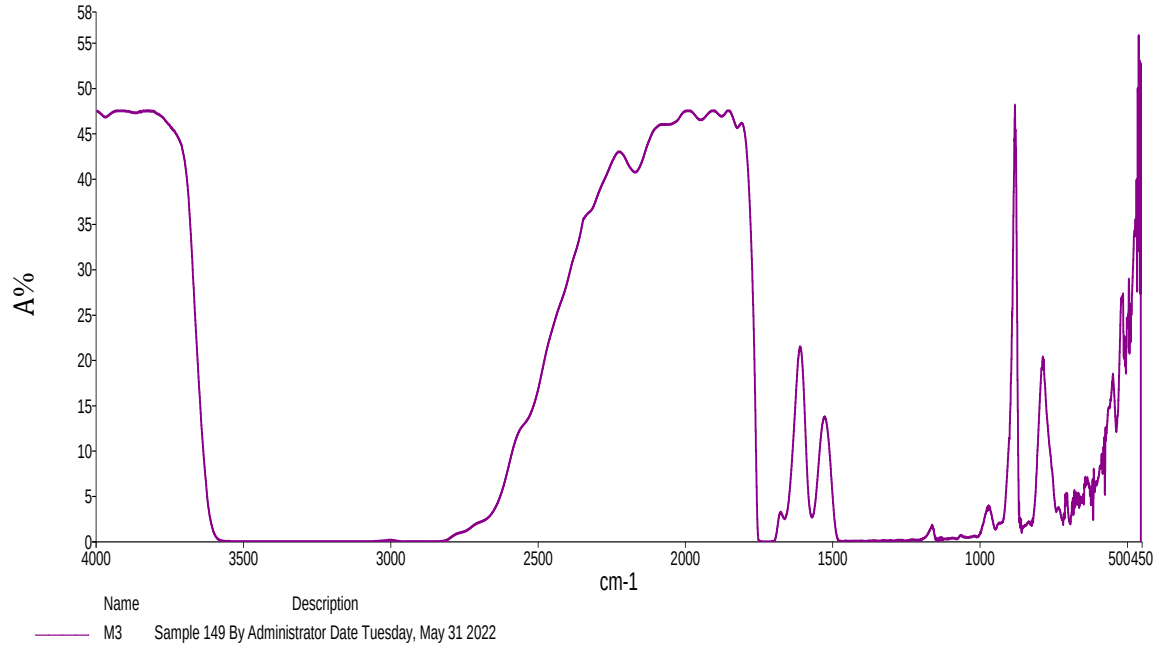
b



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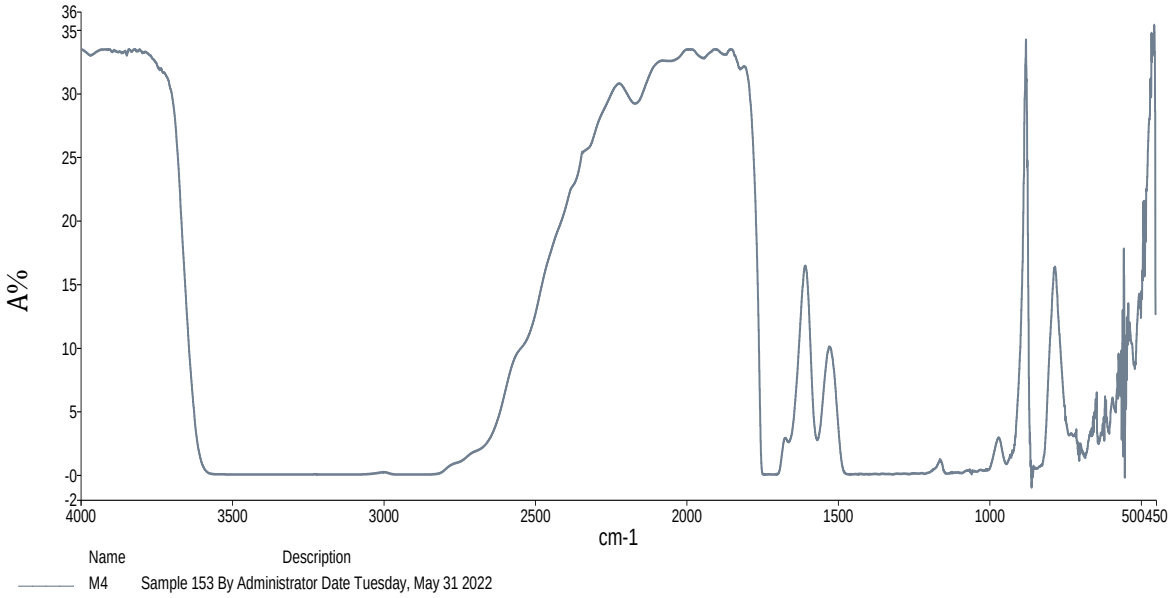


d

Fig. (4.1): FTIR spectra of, a. pure PVA , b. PVA / 3wt.% NiO, c. PVA /5wt.% NiO, d. PVA /7wt.% NiO NC films.

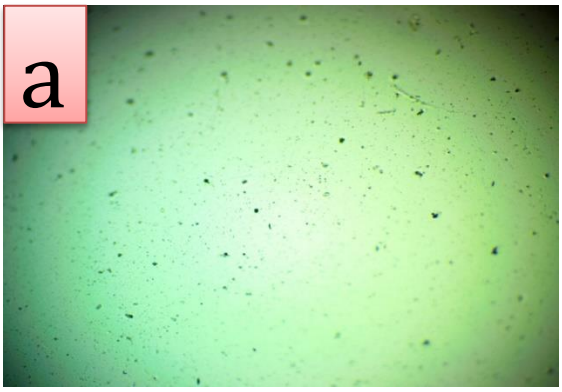
Table (4.1): Experimental values for the wavenumber of the absorption peaks and the corresponding bond.

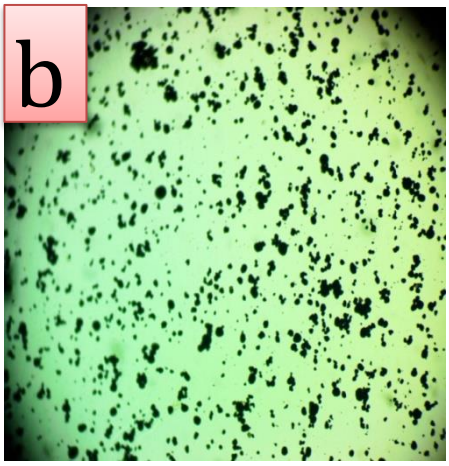
Wavenumber cm^{-1}	Functional Group		Vibration
	PVA	PVA/NiO	
3310.88	O–H	O–H	Hydroxyl group,s stretching (broad)
2903.50	C-H_3	C-H_3	Methyl C-H_3 asymmetric stretching band
2167.08	C≡C	C≡C	medial alkyne (disubstituted)
1724.21	C=O	C=O	Carboylic stretching
1047.38	C-O	C-O	C-O stretching
840.00	C–O–O–	C–O–O–	C–O–O– stretching

4.3 Optical microscopy (OM) of the casting samples

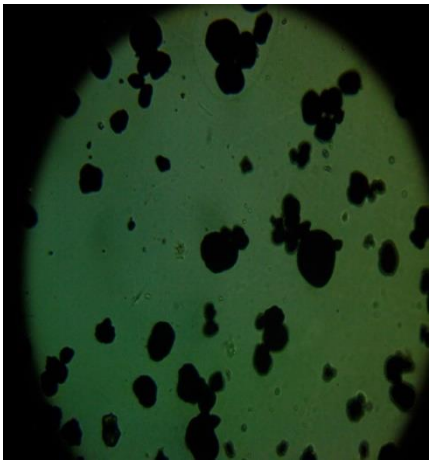
The photomicrographs of the surface of PVA and its **NCs** with different wt.% of NiO NPs at magnification power (10x and 40x) were shown in figure (4.2). The surface image of polymer blend film displayed in part (a) indicates a homogeneous phase without phase separation, in other ward it has a finer morphology with smooth surface. From part b-d, it can be seen, that NiO NPs are well dispersed on the surface of the polymer blend films and this apparent more evident with the increase in the wt.% of NiO. The NCs shows nearly spherical structure of particles. This is because the NPs have a large surface area while the polymeric solution containing different polar groups has a high affinity for NiO which leads to the orientation of the nanoparticles within the

polymer chain and thus the NC structure becomes more compact and thus the consistency of the material increases. This provided a suitable preparation method for preparing NC films[69].

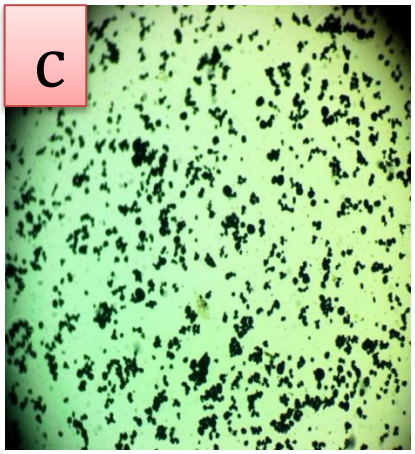




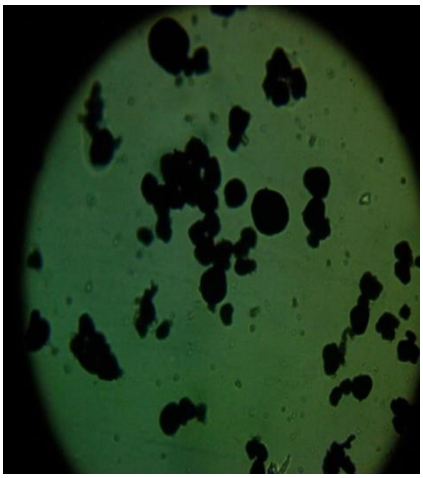
10x



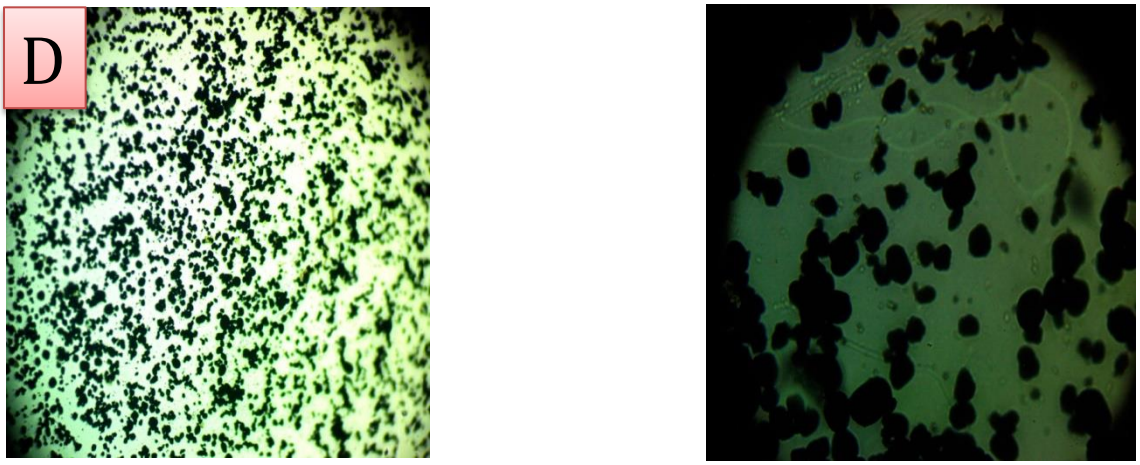
40x



10x



40x



10x 40x

Fig. (4.2): Photomicrographs (10x and 40x) for, a. PVA polymer, b. PVA / 3wt.% NiO, c. PVA / 5wt.% NiO, d. PVA / 7wt.% NiO NCs films.

4.4 The Optical Properties

The main purpose of this study is to identify the effect of adding different wt.% (3, 5 and 7) of NiO NPs on the morphological and optical properties of PVA polymer. The research covers the recording of the spectra of absorbance at RT, knowledge the types of electronic transitions, calculating energy gaps, and optical constants.

4.4.1 Absorbance (A)

Figure (4.3) illustrate the UV-Vis-NIR absorption spectra of PVA and it's NCs with various wt.% of NiO NPs films carried out in the range of 190-1100nm. The absorption edge for NCs films was shifted toward red side with adding NiO, causing a decrease in the energy gap. This may be attribute to the change in polymeric chain mobility during the blending process[70]. It can be seen that the absorption of NCs is much higher than that of blend. The higher absorption of NCs

is attributed to the interfacial interaction between the NPs and the adjacent polar groups of polymer, which were consistent with reported[71].

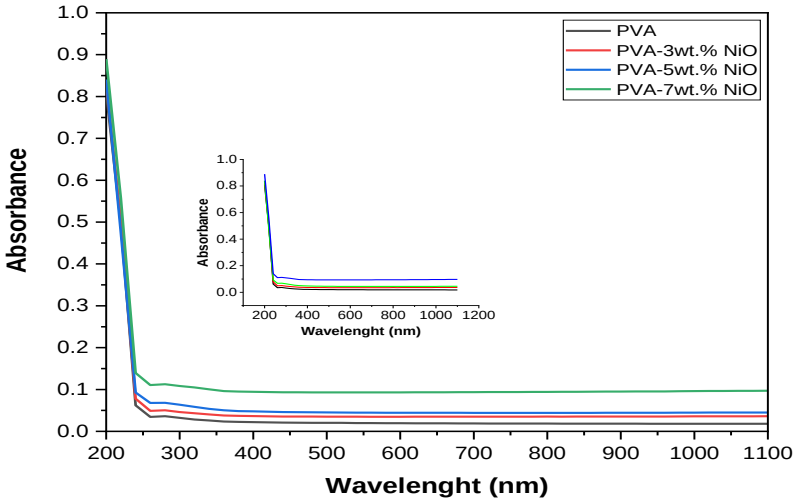


Fig. (4.3) : Absorbance spectra of PVA and its NCs with different wt.% of NiO NPs.

4.4.2 Transmittance (T)

Optical transmittance spectrum of PVA and its NCs with different wt.% of NiO films. Based on the results in figure (4.4), the optimal value of transmittance for pure polymer is about 97-98% in the regions Vis and NIR, but it decreases drastically with an increase in the wt.% Ag NPs. This property was due to the nature of the films surface and its absorption[72].

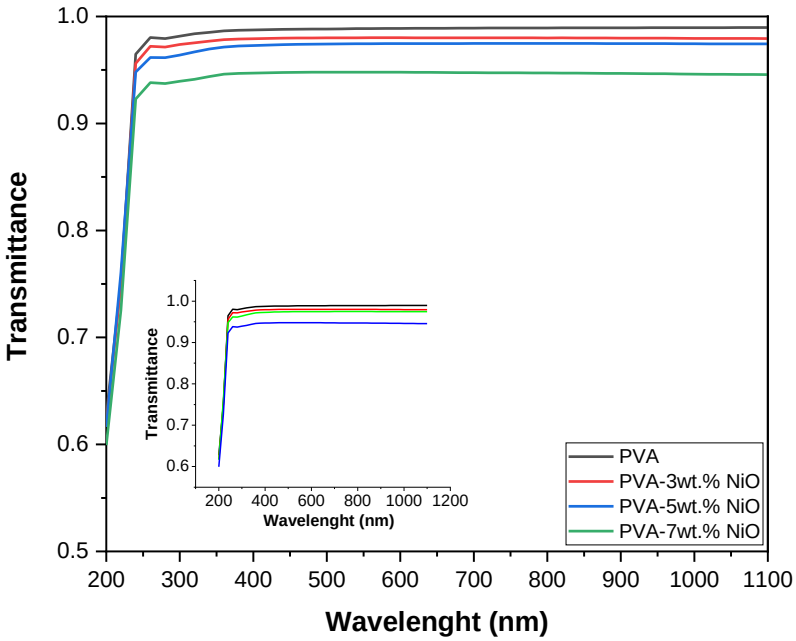


Fig. (4.4): UV-Visible transmittance spectra of PVA and its NCs with different wt.% of NiO NPs.

4.4.3 Absorption coefficient (α)

The absorption coefficient (α) of the blended polymers and its NC films was calculated from Lambert Beer's law (2.3).

Based on the absorption coefficient values of the prepared films ($\alpha < 10^4$ cm^{-1}) as in figure (4.5), indirect electronic transitions are extremely likely to occurs. α look smaller at high photon energy, that could relate to the little possibility of electron transition. The absorption of the electron is at high energies, which is agree with similar studies of NiO NPs [70].

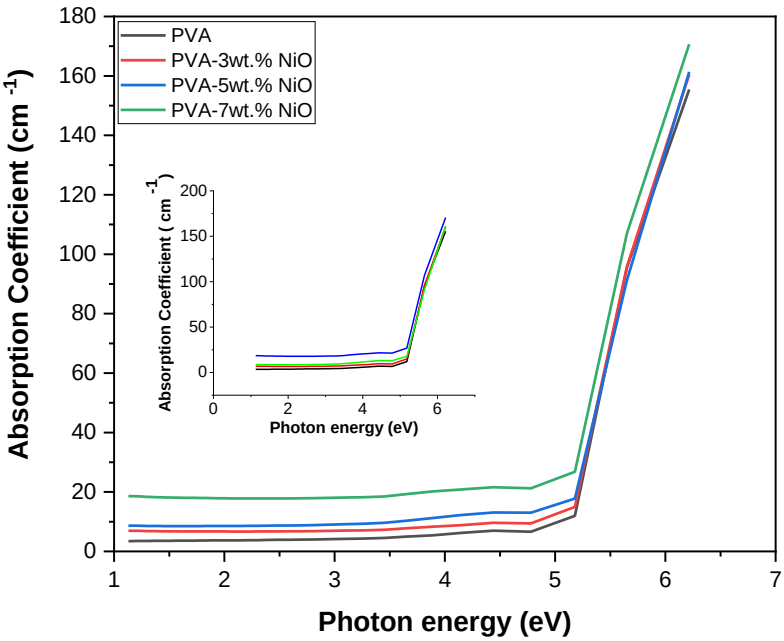


Fig. (4.5): Absorption coefficient PVA and its NCs with different wt.% of NiO NPs.

4.4.4 Optical energy gaps of the allowed and forbidden indirect transition

Depending on the absorption coefficient the optical energy gap can be determined from the plot of $(\alpha h\nu)^{1/r}$ (where r = 2 for allowed and 3 for forbidden indirect transition) versus photon energy (hν) shown in the figures (4.6) and (4.7) using the Tauc relation [2.4] .

The both values allowed and forbidden indirect transitions reduce with additives of NiO NPs which illustrated in Table (4.1)[73].

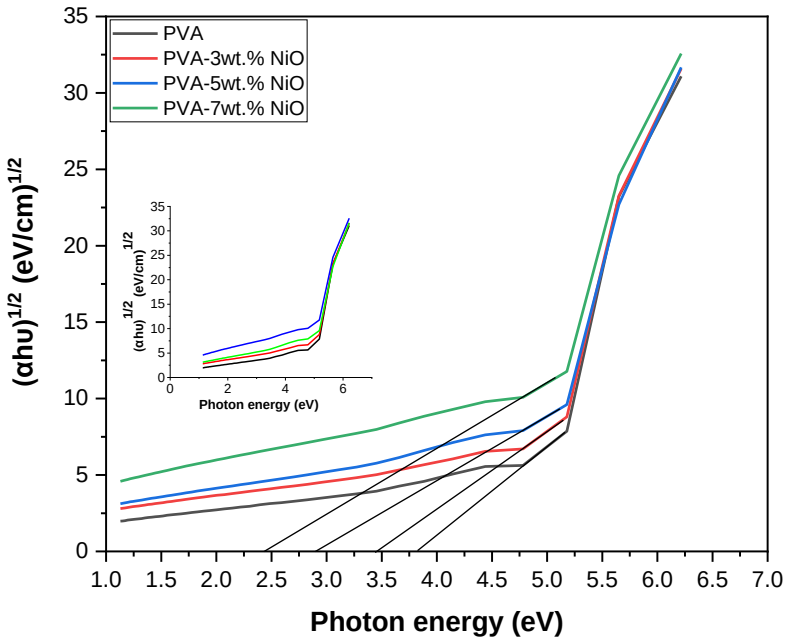


Fig. (4.6): Correlation between $(\alpha h\nu)^{½}$ vs. $(h\nu)$ for PVA and its NCs with NiO NPs.

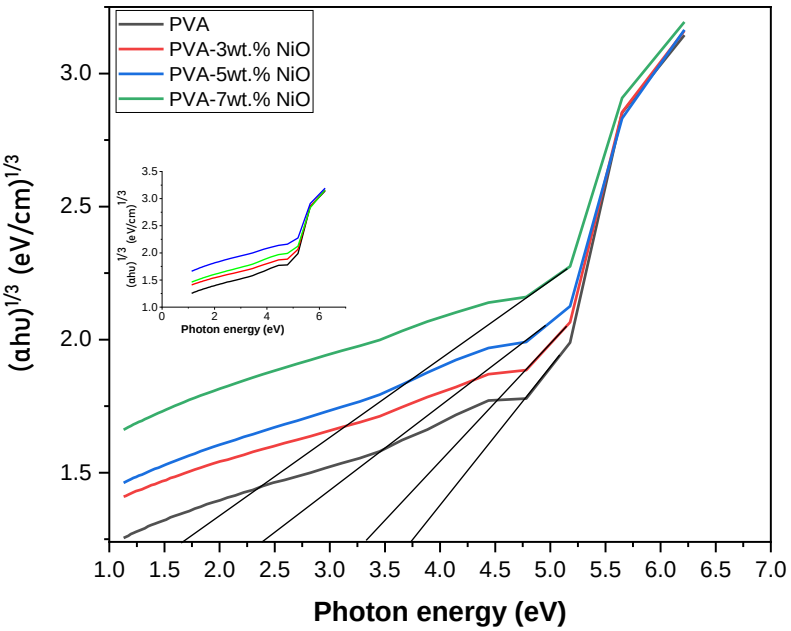


Fig. (4.7): Correlation between $(\alpha h\nu)^{⅓}$ vs. $(h\nu)$ for PVA and its NCs with NiO NPs .

Table (4.2): E_g^{opt} values for indirect transition of PVA and its NCs.

Sample	Allowed (eV)	Forbidden (eV)
PVA	4.85	3.75
PVA / 3wt.% NiO	3.95	3.35
5wt.% NiO	2.9	2.42
5wt.% NiO	2.41	1.71

4.4.5 Refractive index(n) and extinction coefficient (K_o)

The Refractive Index (n) and Extinction Coefficient (K_O) of pure PVA and its nanocomposites with NPs films has been calculated from the eqs. [2.5 and 2.6].

From the figure (4.8), it was found that the NC films is bigger than that of pure PVA in the Vis and NIR regions of the spectrum, due to the large index of NiO[74].

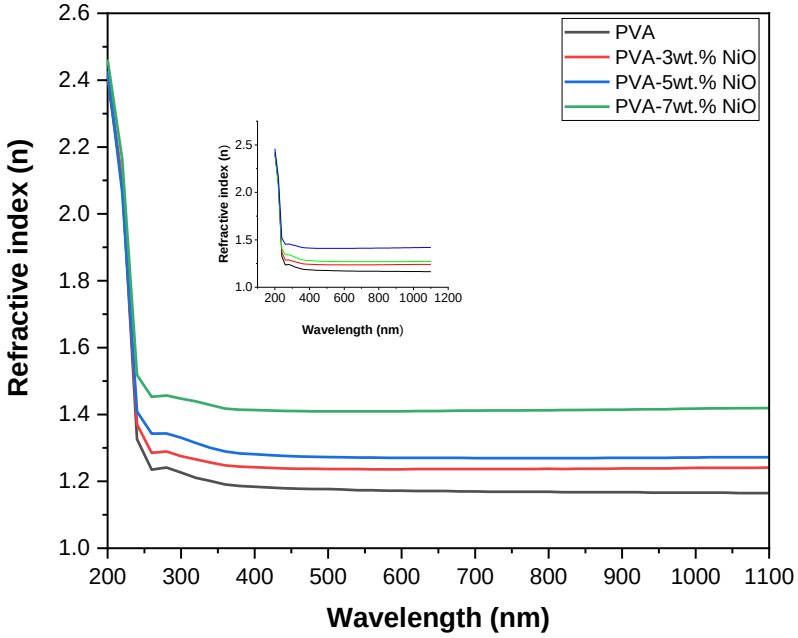


Fig. (4.8): Refractive index (n) of PVA and it's NCs with NiO NPs.

From observation of the figure (4.9), it can be notice that the extinction coefficient results of the NC films are much larger than that of the pure polymer in all regions. This result was directly depended on the absorption of light[75].

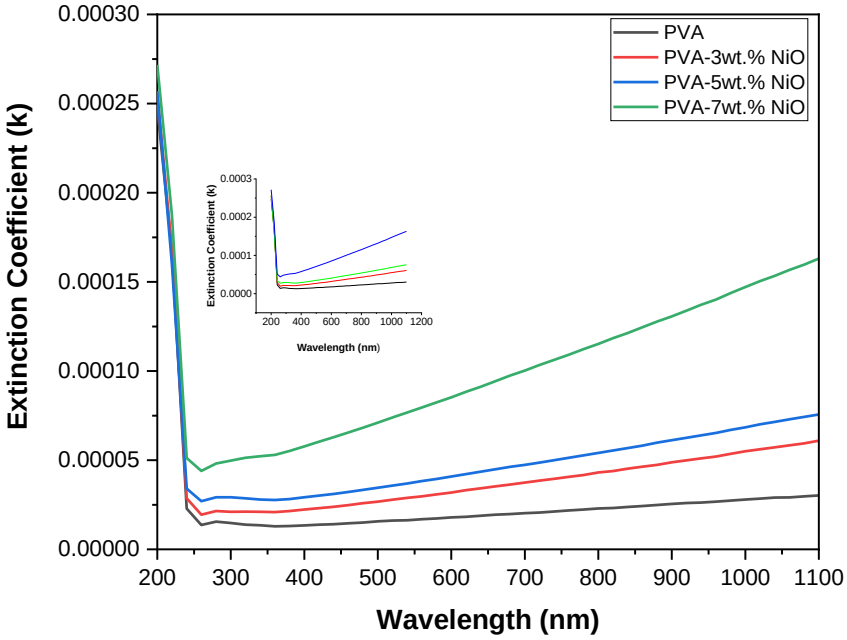


Fig. (4.9): Extinction coefficient of of PVA and it's NCs with NiO NPs

4.4.6 Real and imaginary parts of dielectric constant (ε_r, ε_i)

Figures (4.10) and (4.11) illustrated the variation of real ($\boldsymbol{\varepsilon_r}$) and imaginary ($\boldsymbol{\varepsilon_i}$) parts of the dielectric constant for pure polymer and its NCs with different wt.% of NiO NPs as a function of wavelength. Equations (2.28) and (2.29) were used to obtain the real and imaginary dielectric constants. It can be seen from the figure that ($\boldsymbol{\varepsilon_r}$) considerably dependent on (n^2) due to the low value of (k^2). The real dielectric constant is increased with the increase of NPs. ε_i is dependent on (k) values that are changing with the change of the absorption coefficient due to the relation between (α) and (k) [76].

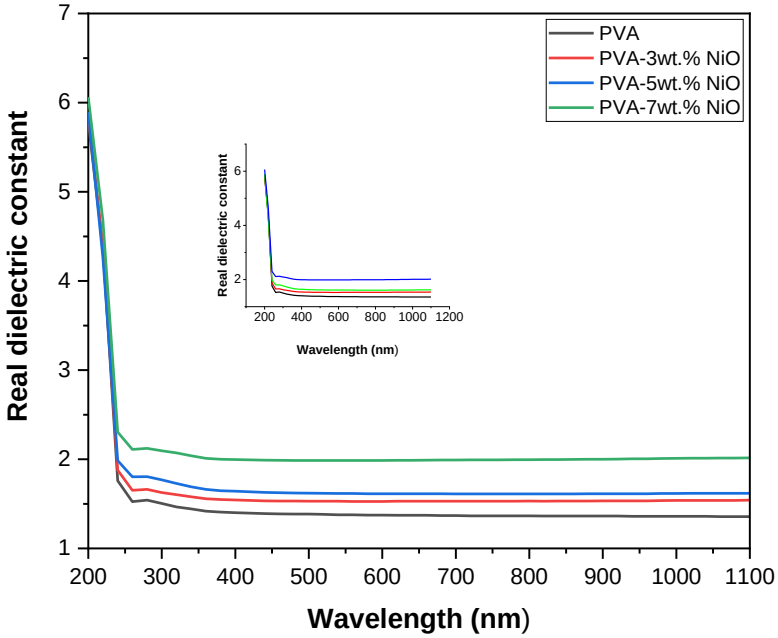


Fig. (4.10): Real dielectric constant of PVA and its NCs with NiO NPs.

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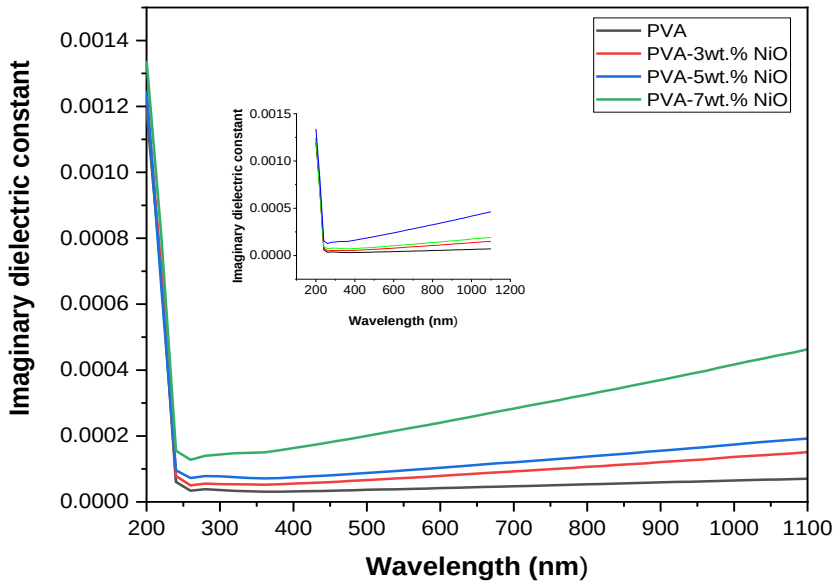

Fig. (4.11): Imaginary dielectric constant of PVA and its NCs with NiO NPs.

4.4.7 Optical conductivity

Figure (4.12) shows the variation of optical conductivity with the wavelength for PVA and its NCs with NiO NPs. The optical conductivity are decreased with the increasing of the wavelength . The increase of optical conductivity at low wavelength of photon is due to high absorbance of all samples in this region, hence, increase of the charge transfers excitations. The optical conductivity spectra indicated that the samples are transmittance within the visible and near infrared regions. Also, the optical conductivity of nanocomposites is increased with the increase of NiO NPs, this behavior is related to the creation of localized levels in the energy gap[68].

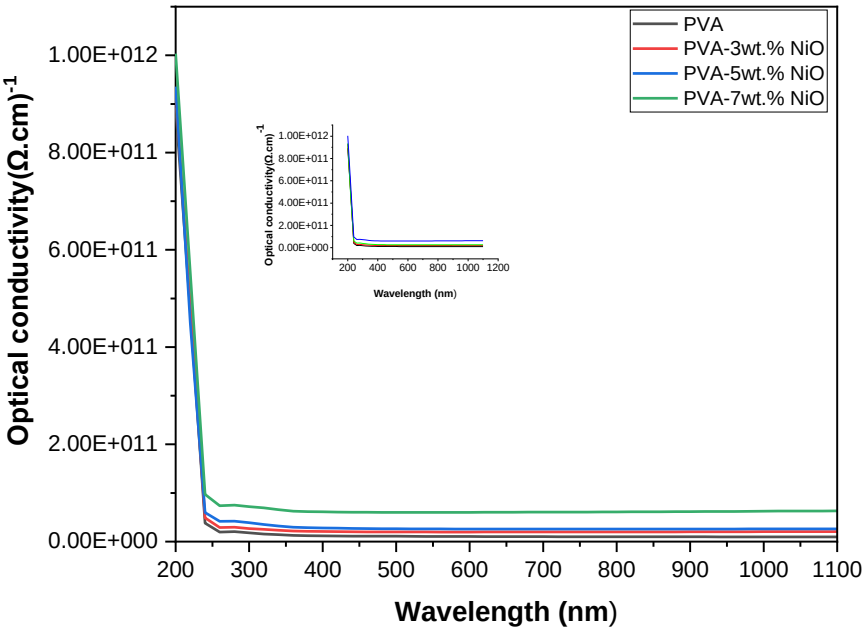

Fig. (4.12). Variation of optical conductivity of PVA and its NCs with NiO NPs.

4.5 Conclusions

From Polymer and its nanocomposite films, it can be concluded:

1. The FT-IR spectra confirmed of the produce the functional groups present in polymer nanocomposite systems, and it was not observed apparent shifting, as a result of the addition of NiO. Also the transmittance decreases with the increasing ratios of NiO NPs that assigned to increase the density of NPs .

2. The photomicrographs of the surface of PVA and its **NCs** with different wt.% of NiO NPs indicates a homogeneous phase without phase separation, in other ward it has a finer morphology with smooth surface, also NiO NPs are well dispersed on the surface of the polymer films and this apparent more evident with the increase in the wt.% of NiO.

3. The absorbance , absorption coefficientr ,refractive index, extinction coefficient, dielectric constant (real, imaginary) and optical conductivity of PVA are increasing with the increasing of NiO nanoparticles concentrations.

4. The optimal value of transmittance for pure polymer is about 97-98% in the regions Vis and NIR

5.The energy gap for indirect transition (allowed, and forbidden) and transmittance of PVA decrease with the increasing of NiO nanoparticles concentrations.

4.6 Future Work

1- Study of the thermal properties of PVA/NiO nanocomposites.

2- Study of the mechanical properties of PVA/NiO nanocomposites.

3- Study of the electrical properties and antibacterial activity application of PVA/NiO nanocomposites.

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الخلاصة

تم تحضير بوليمر PVA ومركباته النانوية ذات الوزن المختلف (٣ و ٥ و ٧ %) من NiO NPs باستخدام طريقة صب المحلول. تم تحديد النتائج بواسطة مطيافية فوريه لتحويل الأشعة تحت الحمراء (FT-IR)، والمجهر الضوئي (OM) ، والتحليل الطيفي للأشعة فوق البنفسجية المرئية. أكدت أطياف FT-IRعلى إنتاج المجموعات الوظيفية الموجودة في أنظمة البوليمر النانوية. تشير الصور المجهرية الضوئية إلى تجانس جيد وتوزيع جيد لـ .NiO NP أظهر التحليل الطيفي للأشعة فوق البنفسجية المرئية أن القيمة المثلى للنفاذية لفيلم البوليمر هي حوالي ٩٧-٩٨٪ في المناطق Vis و NIR ، لكنها تتناقص بشكل كبير مع زيادة في الوزن.٪ .NiO NPsتم تحديد فجوات الطاقة الضوئية غير المباشرة المسموح بها والممنوعة من طيف الامتصاص ، والتي انخفضت قيمها مع زيادة نسب محتوىNiO NPs ، يتزايد الامتصاص ، معامل الامتصاص ، معامل الانكسار ، معامل الانقراض ، ثابت العزل (الحقيقي ، التخيلي) والتوصيل البصري لـ PVA مع زيادة تركيزات جزيئات NiO النانوية.

جمهورية العراق

وزارة التعليم العالي والبحث العلمي

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قسم الفيزياء

تأثير جسيمات أوكسيد النيكل النانوية على الخواص التركيبية والبصرية لبولي فينيل الكحول المصبوب

بحث مقدم

إلى مجلس كلية التربية للعلوم الصرفة في جامعة بابل وهو جزء من متطلبات نيل درجة الدبلوم العالي في التربية / فيزياء المواد وتطبيقاتها.

من قبل الطالب

حسين كامل محمد حسن

بكالوريوس تربية فيزياء

جامعة القادسية ٢٠١٤م

بإشراف

أ.د. فؤاد شاكر هاشم

١٤٤٤هـ ٢٠٢٢م