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Study the Optical Characteristics (PVA-PVP/Sic) Nanocomposites

A research

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بِسْمِ اللَّهِ الرَّحْمَٰنِ الرَّحِيمِ

إِنَّا فَتَحْنَا لَكَ فَتْحًا مُبِينًا (1)

صدق الله العلي العظيم

(سورة الفتح –الاية(1))

Dedication

I dedicate my humble effort to those who helped me facing the difficulties, and gave me everything without limits (my father - my mother - my wife)........

To the candles that lighten the path of knowledge, my teachers…

To the joy of my life (my son).....
To everyone who stands beside me.

Acknowledgments

Praise be to ALLAH, Lord of the Worlds, and praise be to His right and due, and praise him above Hamad Al Hamedin and owe him to the Day of Judgment ... Praise be to God who guided us to science and ridiculed us the doors to understand him and thank him and his prayers and peace be upon His Prophet and on the pure ones.

I would like to extend my thanks and appreciation to Professor Dr.Ahmed Hashim

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My thanks and appreciation to the Deanship of the Faculty of Education for Pure Sciences - University of Babylon and to the head of the Department of Physics to give them the opportunity and their scientific care and their desire to provide a helping hand and help me.

it is also a pleasure to offer my deepest thanks and appreciation to my family for the suffering they have suffered with me throughout the preparation of this letter and their standing with me and their support from my family.

Finally, I extend my sincere thanks, appreciation and respect to my graduate students. I wish them more success and success, and to all those who have spoken to me, even if I have extended a helping hand during my scientific career. May God help everyone.

summary

The polymeric Nano composites of (Polyvinyl Alcohol (PVA) PolyVinyle Pyrrolidone (PVP) - Silicon Carbide (SiC)) were prepared by adding silicon carbide nanoparticles (SiC NPs) with different weight concentrations (0.5,1 and1.5) wt.% the blend of polyvinyl alcohol(PVA) and poly vinyl propylene(PVP) using casting method. The optical properties of (PVA-PVP-SiC) nanocomposites studied at a wavelength (220-820) nm. The results showed that absorbance, absorption of coefficient, extinction coefficient, refractive index, dielectric constants and optical conductivity of (PVA-PVP) blend ware increased while transmittance and energy gap war decreased with increasy SiC NPs content. The (PVA-PVP-SiC) nanocomposites had higher absorption at UV- region. The results of optical properties indicated that the (PVA-PVP-SiC) nanocomposites may be useful for different optical fields.

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List of Symbols

Symbol	Description
A	Absorbance
A	absorption coefficient
C.B	delivery package
E	Electrical Field Intensity
E_{ph}	Photon Energy
E_g^{opt}	Optical Energy Gap
H	Planck constant
I_T	Transmitted Intensity Beam
I_A	Absorbed light Intensity
I_o	Incident Intensity of light
K	Extinction Coefficient

ΔK	change in vector vector
N	refractive index
N	number of polymer molecules
PVA	Polyvinyl Alcohol
PVP	Poly(Vinyle Pyrrolidone)
R	Reflectivity
Sic	Silicon Carbide
T	Transmittance
V.B	parity package
λ	Wavelength of Photon
$\boldsymbol{\sigma}_{\mathbf{op}}$	Optical Conductivity
υ	Frequency
ε_1	Real Dielectric Constant
ε_2	Imaginary Dielectric Constant

Chapter One

Theoretical Part

1.1 Introduction

Nanotechnology is a rapidly developing field because of its wide range of applications in sciences, industries, biotechnology, and nanosciences. The word nanotechnology is generally used when referring to materials of (1-100) nm in size. When a material is reduced to nanosize, it acts differently and exhibits some new properties, which completely lacks in its macroscale or bulk form. Nanoparticles are of great scientific interest, because they bridge the gap between bulk materials and atomic and/or molecular structures[1,2]. Nanoparticles are extremely important because of their exceptionally small size and large surface area to volume ratio, which determines their properties such as electrical, mechanical, chemical, physical, optical, solubility, and stability properties. Generally, nanoparticles are classified into organic and inorganic nanoparticles. Nanoparticles that contain carbon are considered organic nanoparticles whereas metallic nanoparticles, such as noble metal (gold, silver, and platinum) and semiconductor (titanium dioxide, zinc oxide, and zinc sulfide), are considered inorganic nanoparticles[3,4].

1.2 Polymer Structure

Polymers consist of large organic molecules (macromolecules) of repeating small structural units (monomers) connected together in a process called polymerization. Each molecule is composed of thousands of atoms connected by covalent chemical bonds, molecules in a polymer attract each other by forces that depend on the type of the polymer**[5].** Polymers consist of huge, combined molecules. In the solid state, polymers are comprised of crystalline and noncrystalline regions. Crystalline polymers consist of 90% of crystalline regions, while the non-crystalline polymers are almost entirely non crystalline**[6].**

1.3 Nanocomposites

Nanocomposites is a multiphase solid material where one of the phases has one, two or three dimensions of less than 100 nanometers (nm), or structures having nanoscale repeat distances between the different phases that make up the material[7]. The idea behind nanocomposites is to use building blocks with dimensions in nanometer range to design and create new materials with unprecedented flexibility and improvement in their physical properties. Nanocomposites are classified according to matrix materials, as polymer matrix nanocomposites (PMNC), metal matrix nanocomposites (MMNC) and ceramic matrix nanocomposites (CMNC)[8].

Polymeric nanocomposites consisting of inorganic nanoparticles and organic polymers represent a class of materials that have motivated considerable interest in recent years[9]. The nanocomposites applications are quite promising in the fields of microelectronic packaging, medicine, automobiles, optical integrated circuits, drug delivery, injection molded products, sensors, membranes, aerospace, packaging materials, coatings, fire-retardants, adhesives and consumer goods…etc. These advanced nanocomposites have many advantages such as low cost production and the possibility of device fabrication on large scale and flexible substrates[10]. Developing nanocomposites could be a solution to adjust the properties of individual nanomaterial appropriately like, optical, electrical, thermal and mechanical properties. In particular, nanoparticles represent as advanced technological materials because of their attractive electrical / electronic properties and high refractive index. Nanocomposites of organic and inorganic materials can possess advantages of both organic polymers (dielectric, ductility and flexibility) and inorganic materials (high thermal stability, rigidity, strength, high refractive index and hardness), thus have many applications[11].

1.4 The materials Used:

1.4.1 Poly (Vinyl Alcohol) (PVA)

Poly (vinyl alcohol) (PVA) has attracted the attention of many researchers in the reason of their interesting properties such as high dielectric strength, good charge storage capacity, commercial availability, low cost, good mechanical and optical properties**[12].**

PVA present an excellent host material due to its good film morphology, combined with high flexibility. However, these properties are highly susceptible on humidity which reduces the durability and stability of such polymer; it has been mainly used as a dielectric material, membrane, or adhesive because of its high solubility in water**[13].** PVA is a non-toxic, biocompatible synthetic polymer, having good transparency, high dielectric strength, and fast charge transfer at electrode-nanocomposite interface**[14].** Poly (vinyl alcohol) (PVA) is one type of hydrophilic polymer. It's can be mixed with other materials to get a better composite according to its usefulness**[15].**

The significant feature of PVA is semi crystalline nature that is the presence of both crystalline and amorphous regions causing crystal-amorphous interfacial effects which increases the physical properties**[16].** PVA has a carbon chain backbone with hydroxyl groups attached to methane carbon, Figure **(1.1)**

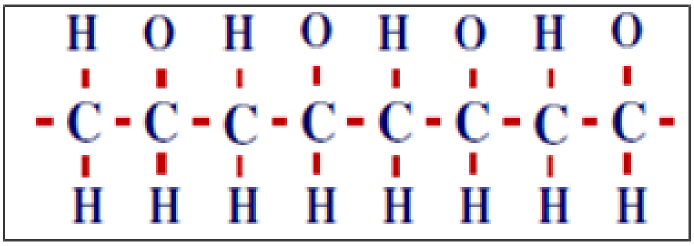


Fig. (1.1). The structure of Poly (vinyl alcohol) [17].

1.4.2 Polyvinyl Pyrrolidone(PVP)

The (PVP) is one of the hydrophilic, biocompatible polymers it is used in many biomedical applications**[18].** and separation processes to increase the hydrophilic character of the blended polymeric materials**[19].** because its solubility in water and its extremely low**[20].** PVP has drawn a special attention amongst the conjugated polymers because its good environmental stability, easy process situation and excellent transparency. PVP is potential, material have a good charge storage capacity and dopant-dependent electrical and optical properties. Chemically, PVP has been bound to be inert, non-toxic and interestingly. It displays a strong tendency for complex formation with a wide variety of smaller molecules**[21].**

1.4.3 Silicon Carbide (SiC)

One of the favorable filter ceramics for high temperature structural components because of its excellent mechanical, electrical and thermal properties such as fracture strength, high elastic modulus, hardness and toughness, relatively low density, chemical stability and good thermal, good thermal conductivity as well as low thermal expansion co-efficient and high resistivity**[22,23].** A blend of SIC with metals/ metal oxides compensates its expands engineering applications and brittleness**[24].** Without addition of any metal or metal oxide as sintering aids, be very difficult to sinter pure form SIC through conventional heating technique because SIC requires a higher temperature above (2000C°) to be sintered. The oxide phase greatly decreases the sintering temperature and improves.

the fracture toughness of the materials**[22,25].** The region of polymer nanocomposites around the nanofillers called interphase, the interphase can have less or more dense structure compared to polymer matrix depending on the interaction between polymer molecules and nanofillers ,figure**(1.2)**

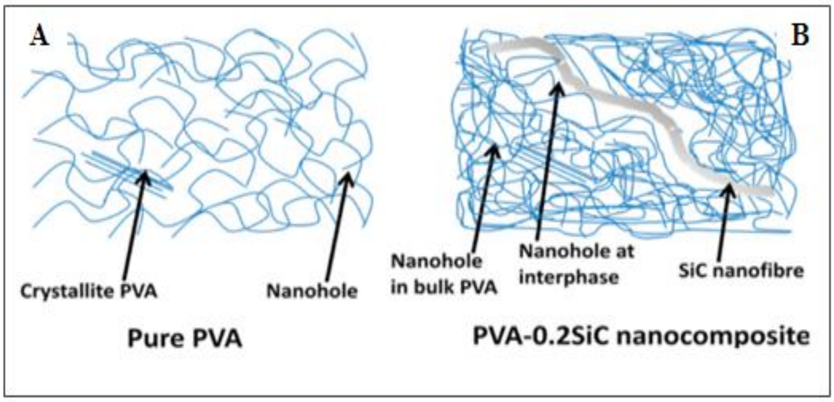


Fig. (1.2). (A) Free volume nanoholes in pure PVA, (B) PVA-SIC nanocomposite structure having two layers [26].

1.5 Literature Review

Nano composites have many medical and industrial applications. Previous research has examined and optical properties, their applications to various compounds and nanoparticles

Gao, H., & Lian, K. al. [27] in (2013) were studied the effects of nano-SiO_2 and nano-TiO_2 fillers on a thin film silicotungstic acid (SiWA)−H3PO4−poly(vinyl alcohol) (PVA) proton conducting polymer electrolyte and compared with respect to their proton conductivity, environmental stability, and dielectric properties. Dielectric analyses were used to differentiate these effects on polymer electrolyte-enabled capacitors. Capacitor performance was correlated to electrolyte properties through dielectric constant and dielectric loss spectra. Using a single-ion approach, proton density and proton mobility of each polymer electrolyte were derived as a function of temperature. The results allow us to deconvolute the different contributions to proton conductivity in SiWA−H3PO4−PVA-based electrolytes, especially in terms of the effects of fillers on the dynamic equilibrium of free protons and protonated water in the electrolytes.

Ma, H.et al. [28] in (2014) were prepared PVA/SiO_2-TiO_2 hybrid fibers by sol-gel dip-coating method. PVA and SiO_2-TiO_2 were linked through chemical bond in the hybrid fiber, and forms a homogeneous system. There was a comparing with pure PVA fiber, They found that the crystallinity of hybrid fibers decreased dramatically and the hybrid fibers shield the ultraviolet rays effectively by adding TiO_2, and this could slow the elderly process of the PVA/SiO_2 hybrid materials, and too the thermal resistance of hybrid fiber is better than pure PVA fiber. The resulting PVA/SiO_2-TiO_2 hybrid materials might be very promising for use in ultraviolet radiation shield fibers due to the ultraviolet radiation shield effect of TiO_2.

C. G. A. Beltran and *et al.*[29] in (2015) were investigated the structural and optical properties of (PMMA-ZrO_2) nanocomposites using sol-gel method to deposit homogeneous and highly transparent on glass substrates. SEM and AFM images of the hybrid films show a uniform, smooth, and very flat surface with average roughness lower than 1 nm. The cross-sectional image shows also transversal homogeneity and thickness uniformity. The thickness, refraction index (at 532 nm), and optical band gap of the hybrid films, as determined from T and R spectroscopy measurements were 440 nm, 1.57 (at 532 nm) and 4.46 eV, respectively.

E. H. Alsharaeh[30] in (2016) study the preparation of nanocomposites of (PS), (PMMA), and PSMMA co-polymer containing (Ag NPs) using in situ bulk polymerization with and without microwave irradiation (MWI). The Ag NPs prepared were embedded within the polymer matrix. FTIR and XPS studies confirmed the formation of metallic Ag NPs within the polymer matrix. UV-Vis spectra of the PS/Ag and PMMA/Ag nanocomposites revealed a red shift with respect to the PSMMA/Ag nanocomposites, confirming the size effect of Ag NPs.

A. Goyal and *et al.*[31] in (2017) were investigated the optical and electrical properties of (Ag-PMMA) nanocomposites films were prepared via ex situ chemical route by employing sodium borohydride ($NaBH_4$) as a reducing agent. The alteration in optical and structural performances of PMMA was established by UV-visible spectroscopy, SEM and Raman spectroscopy. It is observed that the concentration of Ag nanoparticles has strongly influenced the optical, structural and electrical properties of PMMA matrix. The increase in the electrical conductivity and the increase in Urbach's energy Eu value from 0.40 to 1.11 eV with increase in the concentration of Ag nanoparticles in PMMA matrix can be correlated to the formation of the localized energy states within HOMO-LUMO gap of PMMA matrix.

V. S. Esha and *et al.*[32] in (2018) were presented a theoretical investigation on the application of density functional theory calculations of optical and thermodynamic properties of the Poly (Methyl MethAcrylate) polymers (PMMA or nMMA; n = 1 to 5). Also, a sequential red shift in the spectra during the growth of the polymer addresses the suitability of visible active nature of PMMA at larger dimension as reported in recent experimental studies. The linear response of ($\alpha^{1/3}$) with the inverse of I_P indicates that PMMA polymerization obeys the minimum polarizability principle. The thermodynamic properties, viz., S, H and G also favor the polymerization process.

S. Ahmed and *et al.*[33] in (2019) were investigated the influence of thickness on the optical properties for poly methyl methacrylate (PMMA), that the films were prepared by spin coating method. Some of optical properties of poly(methyl methacrylate) film have studied, this study shows that having different properties due to the difference in thickness. The measurements were taken for different thickness (206,116,87,66,47 nm) and different number of rotation (1000,2000,3000,4000,5000 rpm) respectively. Note that the value of optical measurements have been measured (absorption, refractive index, reflectance and real dielectric constant) behave the same behavior, while the (transmittance, extinction coefficient, absorption, coefficient and imaginary dielectric constant) behave the same behavior due to the impact of thickness. Effect of thickness variation and number of rotation on optical measurements. Also notice the value of the energy gap is as high as possible and reaches to (3.08 eV) at 5000 rpm with thickness (47 nm) and have the highest refraction at the value that the thickness(206 nm).

S. A. Hussain and ***et al.*****[34] in (2020**) were studied the effect of nanoparticle of Silver on the optical properties of Polymethylmethacrylate (PMMA) films prepared by using casting technique at a temperature (50 C°) with thickness (8±1 μm). The optical properties of the composite were done by measuring the absorption and transmission spectra as a function of wavelength (200-800 nm). The results of measurement showed that the transmittance of the films decreased with increasing the addition of silver nanoparticle due to increasing of attenuation of incident light with a clear increase of absorption and a decrease in optical reflectivity. As well as calculated the optical constants (α, k and ε_r) of the prepared films. The results showed an increase when increasing addition.

Dhatarwal P, Sengwa RJ. (2021) Investigation on the optical properties of (PVP/PVA)/Al2O3 nanocomposite films for green disposable optoelectronics. Phys B.

Heiba ZK, Bakr Mohamed M, Ahmed SI. Exploring (2022) the physical propertiesn of PVA/PEG polymeric material upon doping with nano gadolinium oxide. Alexandria Eng J.

1.6 The Aims of Project

This work aims to:

1- The optical properties of (PVA- PVP -SiC) nanocomposites will be studied.

2- Preparation of (PVA- PVP -SiC) nanocomposites to use in a wide variety of biomedical and industrial applications.

Chapter Two
Theoretical Part

2.1 Introduction

Nanocomposites of organic and inorganic materials can have advantages of both organic polymers (ductility, dielectric, flexibility) and inorganic materials (high thermal stability, rigidity, strength, high refractive index, hardness), thus have many applications**[35].**

There is increasing research in nanocomposites owing to improvements in, optical, electrical, mechanical properties. Nanoparticles represent as advanced technological materials because of their attractive electrical/electronic properties and high refractive index**[36,37].**

This chapter contains a theoretical part which effort on the theories of conduction, polarization and optical properties.

2.2The Optical Properties

In recent years, the search for optical properties has increased because of their applications in integrated optics such as optical information, optical data storage, and optical modulation. The study of optical absorption useful for clarification of the electronic structure and determine direct and indirect transitions**[38].**The addition of nanoparticles in polymer improves the optical, electrical and mechanical properties of the materials. Metal oxides nanoparticles with polymers studied as alternative materials for optical applications such as micro optical elements and planar waveguide devices. The developments of polymer nanocomposite structures due to their ease of processing and production, light weight, good adhesion with reinforcing elements, resistance to corrosive environment and in some cases ductile mechanical performance **[39,40].**

2.2.1 Absorbance (A)

Absorbance can be described as the ratio between absorbed light intensity (I_A) by material and the incident intensity of light (I_o) **[41].**

$A=I_A/I_o$ (2.1)

2.2.2 Transmittance (T)

It is determined by the proportion of the intensity of the rays (I_T) that transmits to the of the incident sunlight (Io) intensity as follows through the film **[42].** :

$T = I_T / I_o$ (2.2)

2.2.3 The Absorption Regions

There are three different types of absorption zones **[43].**

i. The magnitude of the absorption coefficient in the high absorption field (α) is greater than or equal to (10^4 cm^{-1}).

ii. The absorption coefficient value in the exponential field (α) is equal to ($1\ cm^{-1} < \alpha < 10^4\ cm^1$).

iii. The absorption coefficient in the low absorption field. (α) is incredibly small, measuring only around ($\alpha < 1cm^{-1}$) as shown in figure (2.1) which shows the absorption regions

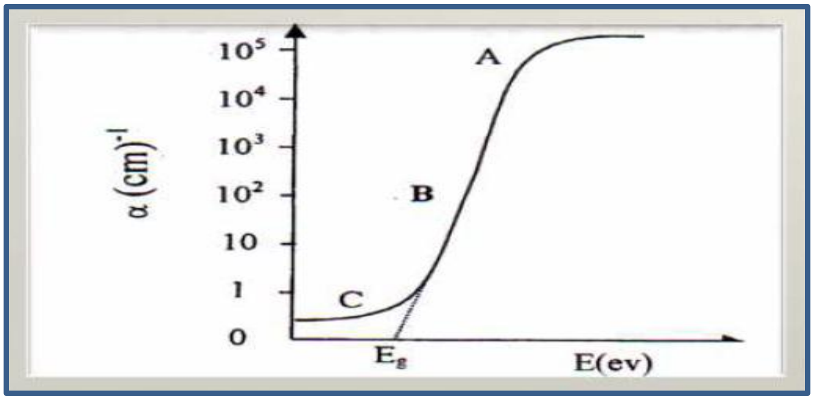


Figure (2.1). The absorption regions[43].

2.2.3 Fundamental Absorption Edge

The fundamental absorption edge can be defined as the rapid increasing in absorptance w

hen 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 **[44].** , absorption regions can be divided into three regions **[45].** :

A) High absorption Region

This region is shown in Figure (2.1). In part (A), the magnitude of absorption coefficient (α) is larger or equals to (10^4 cm^{-1}). This region can be introduced to magnitude the forbidden optical energy gap ($E_g^{opt.}$).

B) Exponential Region

This region is shown in Figure (2.1). In part (B), the value of absorption coefficient (α) equals to ($1\ cm^{-1} < \alpha < 10^4\ cm^{-1}$). It refers to the 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

This region is shown in Figure (2.1). In part (C), 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.

2.2.5 The Electronic Transitions

There are two basic types of electronic transition ,direct and indirect transition :

1. Direct Transitions

This transition happens in semiconductors when the bottom of conduction band is exactly over the top of valance band,this means that they have the same value of wave vector i.e. ($\Delta K=0$). In this case, the absorption will appear at ($h\upsilon=E_g^{opt.}$). Therefore, the phonons do not take part in direct transition because the wave vector (K) of the phonon is much larger than that of the photons. This transition type requires the laws of conservation in energy and momentum . Therefore the direct photon transition at the energy of the minimum gap cannot satisfy the requirement of conservation of wave vector because photon wave vectors are negligible at the energy range of interest**[46].** These direct transitions have two types**[47].**

A- Direct Allowed Transition :

This transition happens from the top points in the valance band and the bottom point in the conduction band , as shown in Figure (2.2-a).

B- Direct Forbidden Transitions:

This transition happens from the near top points of valance band and the bottom points of conductive band, as shown in Figure (2.2-b).

The absorption coefficient for this transition type is given by **[48].**:

$$\alpha h\upsilon=B\ (h\upsilon-E_g^{opt.})^r \qquad (2.3)$$

Where: $E_g^{opt.}$ energy gap between direct transition.
B: constant depended on type of material.
r: exponential constant, its value depended on type of transition,
r =1/2 for the allowed direct transition.

r =3/2 for the forbidden direct transition.

2. Indirect Transitions

In these transitions type, the bottom of conductive band is not over the top of valance band. The electron transits from valance band to conductive band 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 particle called "Phonon", for conservation of the energy and momentum law. There are two types of indirect transitions **[49].** they are:

A - Allowed Indirect Transitions :

These transitions happen between the top of valance band and the bottom of conductive band which is found in the difference region of (K-space), as in Figure (2.2-c).

B- Forbidden Indirect Transitions :

These transitions happen between near points in the top of valance band and near points in the bottom of conductive band , as shown in Figure (2.2-d).

The absorption coefficient for transition with a phonon absorption is given by **[50]. :**

$$\alpha h\upsilon = B\,(h\upsilon - E_g^{opt.} \pm E_{ph.})^r \qquad (2.4)$$

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.

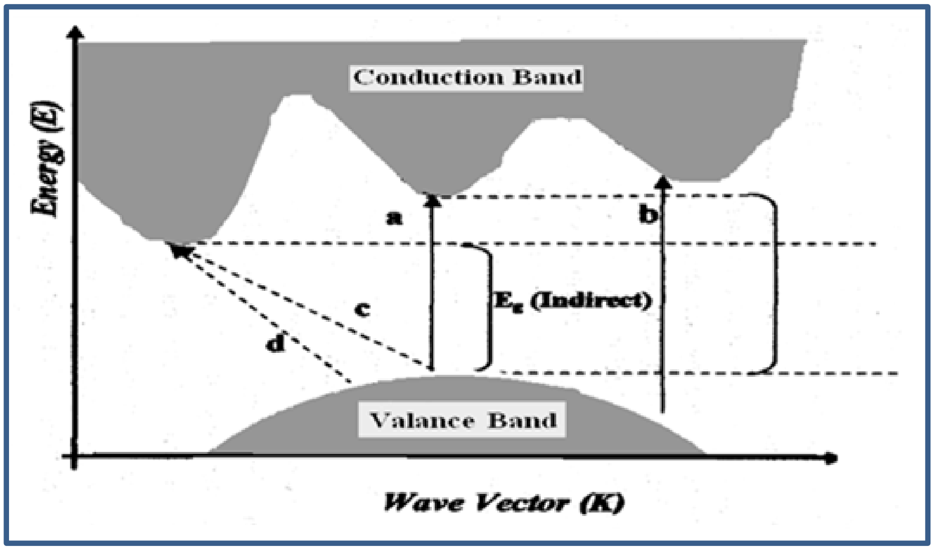


Figure (2.2): The transition types (a- allowed direct transition, b- forbidden direct transition, c- allowed indirect transition, d- forbidden indirect transition)[49].

2.2.5Optical Constant

The study of the optical constants of a material is interesting for many reasons. Firstly, using the materials in optical applications such as interference filters, optical fibers, and reflective coating require accurate knowledge of their optical constants over a wide range of wavelengths. Secondly, the optical properties of all materials may be related to their atomic structure, electronic band structure and electrical properties **[51].**

2.2.5.1 Absorption Coefficient (α)

Absorption coefficient is defined as a ratio decrement in flux of incident rays energy relative to the distance unit in the direction of incident wave diffusion. Absorption coefficient (α) depends on incident photon energy (hυ) and on semiconductor characteristics (n or p) type, where electronic transitions type (n) or (p) and forbidden energy gap. Photon energy is given by the following equation **[52].**

$$E = h\upsilon \qquad (2.5)$$

When incident photon energy is less than forbidden energy gap, then photon will be transmitted, and transmittance gives the following equation **[53].**

$T= (1-R)^2 \exp(-\alpha d)$ (2.6)

Where : T : transmittance, R : is the reflectance.

If the light of intensity (I_o) incident on the film of thickness (d), the transmitted intensity (I_T) can be given as **[47].**

$I_T = I_o \exp(-\alpha d)$ (2.7)

$I_T / I_o = \exp(-\alpha d)$ (2.8)

where : $T = I_T / I_o$

$T = \exp(-\alpha d)$ (2.9)

$1/T = \exp(\alpha d)$ (2.10)

Then:

$\alpha d = 2.303 \log (I_o / I_T)$ (2.11)

But $A= \log (I_o / I_T)$

$\alpha d = 2.303 \times A$ (2.12)

$\alpha = (2.303 \times A) / d$ (2.13)

Where: d is the sample thickness in cm , A is the absorption of the material.

2.2.5.2 Refractive Index (n)

The refractive index can be defined as a ratio between velocity of light in vacuum (C), to its velocity inside the material. The value of refractive index (n) was calculated by using equation (2.16) depending on the reflectance (R) and extinction coefficient (k), as in the following equation **[53].** :

$R= \frac{(n-1)^2 + k^2}{(n+1)^2 + k^2}$ (2.14)

Where: R: is the reflectance and (k) is the extinction coefficient.

Reflectivity can be obtained from absorption and transmission spectrum in accordance with the law of conservation of energy by the relation **[54].** :

$$R + A + T = 1 \tag{2.15}$$

The value refractive index(n) can be calculated by the following equation **[55].**

$$n = \sqrt{\frac{4R - k^2}{(R-1)^2}} - \frac{(R+1)}{(R-1)} \tag{2.16}$$

2.2.5.3 Extinction Coefficient (k)

The imaginary part of the complex refractive index N is called the extinction coefficient, as shown in the following equation **[56].** :

$$N = n - i\,k \tag{2.17}$$

N: is complex refractive index which depends on the material type, crystal structure (grain size), crystal defects, stress in crystal .In addition, the extinction coefficient (k) is given by fallowing equation **[56].** :

$$k = \frac{\alpha\,\lambda}{4\pi} \tag{2.18}$$

Where λ : is the wavelength of incident photon rays

2.2.5.4 Dielectric Constant (ε)

The dielectric constant represents the ability of the matter for polarization. The matter can respond to different frequencies in a complex manner. At optical frequencies represented by light waves the electronic polarity is dominating above other remaining types of polarization. The following equation can calculate the real and imaginary dielectric constant **[57].** :

$$\varepsilon = \varepsilon_1 - i\,\varepsilon_2 \tag{2.19}$$

Where: ε is the complex dielectric constant and (ε_1, $i\varepsilon_2$) are the real and the imaginary parts of the dielectric constant, respectively. The real and imaginary parts of the dielectric constant related to the values and the dielectric constant (ε) can be calculated from refractive index (n), joining complex dielectric coefficient (ε) with complex refractive index (N), as in the following equation **[58].**

$$\varepsilon = N^2 \qquad (2.20)$$

$$(n - i\,k)^2 = \varepsilon_1 - i\,\varepsilon_2 \qquad (2.21)$$

Real and imaginary complex dielectric coefficient can be given as following **[59].**:

$$\varepsilon_1 = (n^2 - k^2) \qquad (2.22)$$

$$\varepsilon_2 = (2nk) \qquad (2.23)$$

2.2.5.5 Optical Conductivity (σ_{op})

The optical conductivity (σ_{op}) depends directing on the refractive index (n) and absorption coefficient (α), according to the following relation **[60].**

$$\sigma_{op} = \frac{\alpha n c}{4\pi} \qquad (2.24)$$

Chapter Three
Experimental Part

3.1 Introduction

This chapter includes the stages of samples preparation and testing measurement stages in addition to a description of the equipment and tools used in the preparation and measurement processes.

3.2 The Materials Used in This Work

The polymer is used in this work:

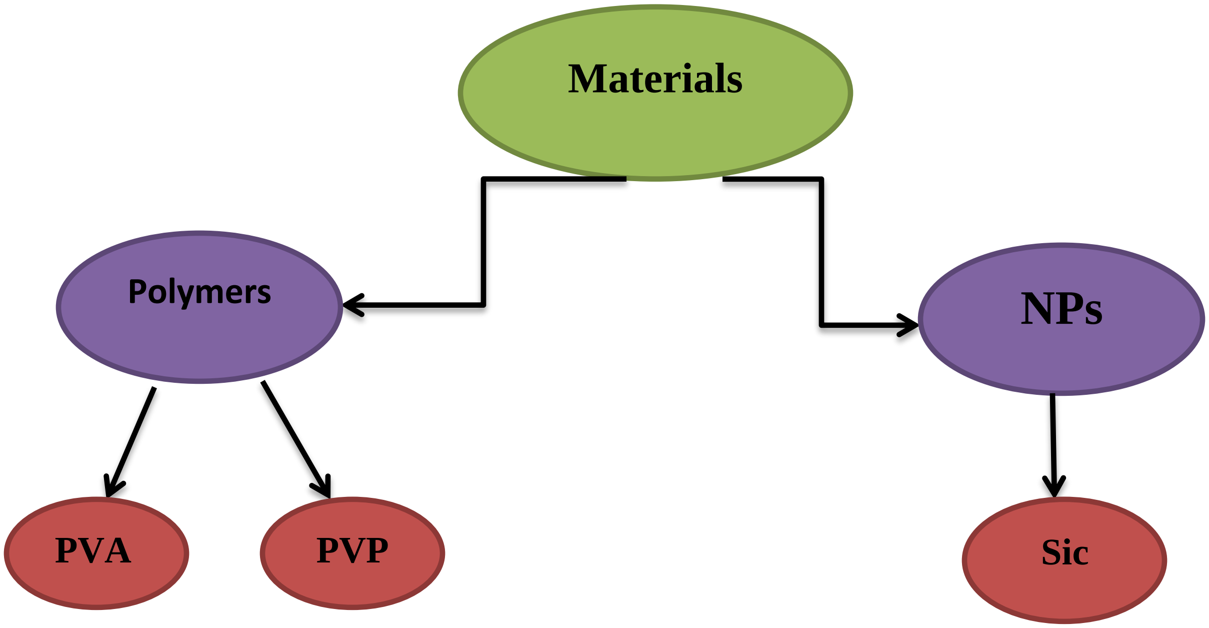
3.2.1Poly(Vinyl Alcohol) (PVA): The polymer is used as granular form and could be obtained from local markets, and high purity (99.98 %).

3.2.2 Poly(Vinyle Pyrrolidone) (PVP)

The material Poly(Vinyle Pyrrolidone) (PVP) used is a white powder, its density is 1.04 g/cm³. It could be obtained from local markets, and high purity (99.99 %).

3.2.3 Additive Nanomaterial

One type of additive nanomaterial was used in this work is Silicon Carbide (SiC) it was obtained as powder from US Research nanomaterials, Inc, USA with size (<80nm,cubic) and high purity (99.%).



3.3 Preparation of samples

The polymeric blend were prepared by dissolving (0.77 g) of polyvinyl alcohol with (0.23 g) polyvinyl pyrrolidone in a (50 ml) of distilled water using a Magnetic Stirrer to a homogeneous solution at a temperature of 85 °C, then adding the weight percentages (0.5,1,1.5)wt% of the Sic nanoparticles

method was used to prepare films onto plastic petri dish bases with a diameter of (5 cm) then left to dry at room temperature.table 1 shows the weights of PVA,PVP,Sic,NPS

Table (1- 3) Weight Percentages of nanocomposites. (PVA,PVP,Sic,NPS)

PVA	PVP	SIC
0.77	0.23	0
0.759	0.227	0.005
0.749	0.224	0.01
0.739	0.221	0.015

3.4 Optical Properties Measurements For Nano composites

The optical properties of (PVA-PVP-SiC) Nano composites are measured by using the double beam spectrophotometer (Shimadzu, UV-1800^{0}A) in wavelength (220-800) nm.

Figure (3.1): UV Photographic of Spectrophotometer.

Chapter Four

Results

&

Discussion

4.1Introduction

This chapter includes the results of optical measurements of (PVA-PVP-SiC) composites prepared by casting method and discusses the results of the effect of adding silicon carbide with different concentrations to the pure mixture (PVA-PVP).

4.2 Optical measurements

The study of the optical properties of Nano composites (PVA-PVP-SIC)is to determine the effect of adding silicon carbide on the optical properties of a mixture of polyvinyl alcohol and poly vinyl propylene..

4.2.1 Absorbance (A)

Figure (4-1)shows the variation of absorbance with photon wavelength for (PVP-PVP-SiC) nanocomposite .the absorbance of (PVA-PVP)blend increase with an increase of SiC NPS content this is due to the density of the localized levels formed by the impurity atoms in the similar material between the valence and conduction bands, as these levels act as auxiliary levels for the transfer of electrons absorbing photons with lower energies. (0.5) wt % also to increase due to a net work formation of the nanoparticle inside the pure polymers **[61].**

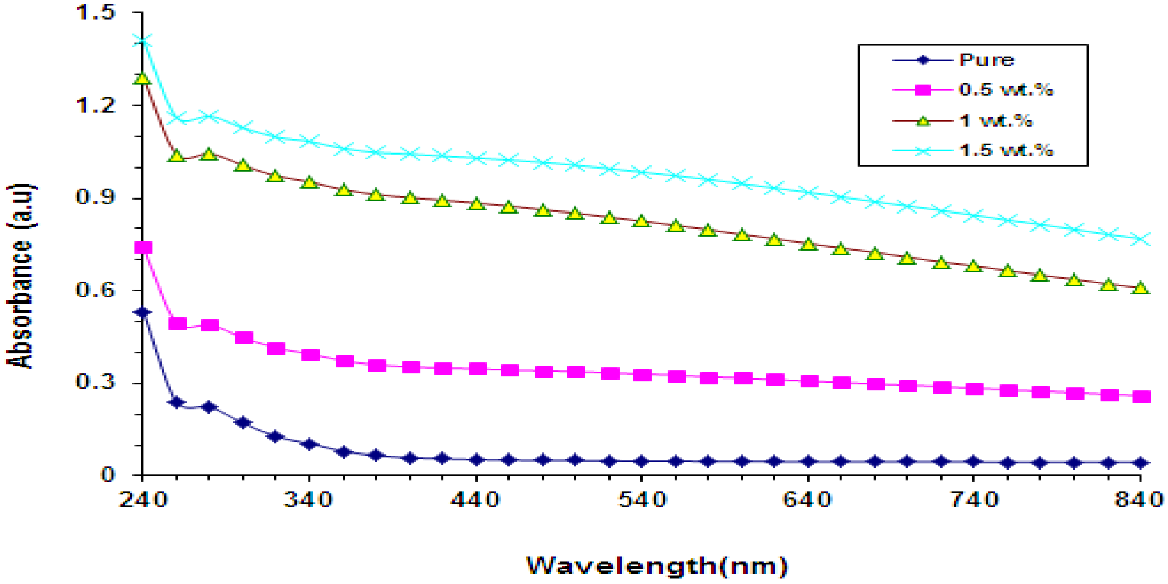


Figure (4-1) the absorbance as a function of the wavelength of (PVA-PVP) films doped with silicon carbide Nps

4.2.2 Transmittance(T)

The transmittance spectrum is characterized by the opposite behavior of the absorbance spectrum, as Figure (4-2)

Transmittance spectrum as a function of the wavelength of (PVA-PVP) films of pure and pure polymer doped silicon carbide NPS The transmittance increases in general with the increase in the wavelength of the electromagnetic radiation falling on the film material, at a high wavelengths . The absorbance spectrum of the (PVA-PVP) films quickly begins to gradually decrease with the increase in the doping ratios taken, due to the impurity atoms and the accompanying formation of local levels within the forbidden energy gap between the valence and conduction bands, and the decrease in absorbance and increase in absorption. The decrease in absorbance is also due to the nature of refractions and reflections within the material itself. As for the pure polyvinyl alcohol and poly vinyl propylene, it finds that they have a high absorbance due to the lack of free electrons, that is, the bonding of electrons to atoms with covalent bonds is due to the breaking of the electrons bond and transferring them to a bundle Conduction requires high-energy photons**[62].**

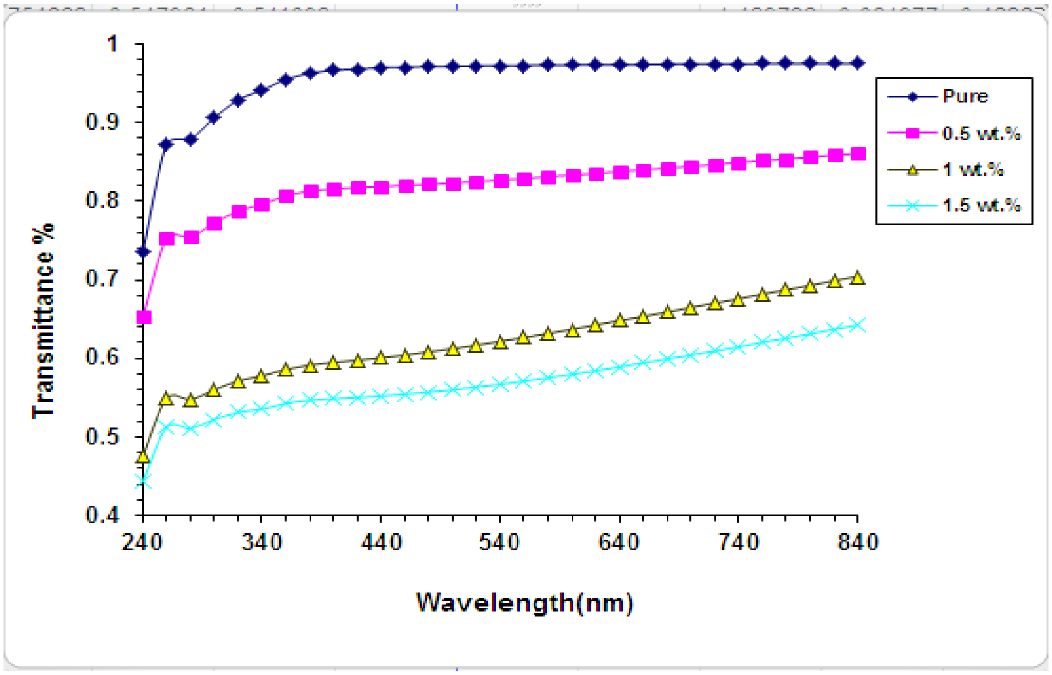


Figure (4-2) The transmittance change (T) of the PVA-PVP-SiC) nanocomposites with wavelength and for different concentrations of SiC.

4.2.3The Absorption coefficient (α)

The absorption coefficient was calculated for (PVA-PVP-SiC)nanocomposite using equation (2-13). The absorption coefficient as a function of the photon energy is shown in Figure (4-3).deduce the nature of electronic transitions, when the values of the absorption coefficient are high ($\alpha>10^4$) cm^{-1} at high energies, direct electronic transitions occur and that the energy and momentum are conserved by electrons and photons, but when the values of the absorption coefficient are low ($\alpha<10^4$) cm^{-1} Indirect electronic transitions occur and the conservation of electronic momentum will be with the help of the phonon. From the results we note that the absorption coefficient of the added complexes (PVA-PVP-SiC) is less than(10^4) cm^{-1}, and this explains that the electronic transitions are indirect**[63].**

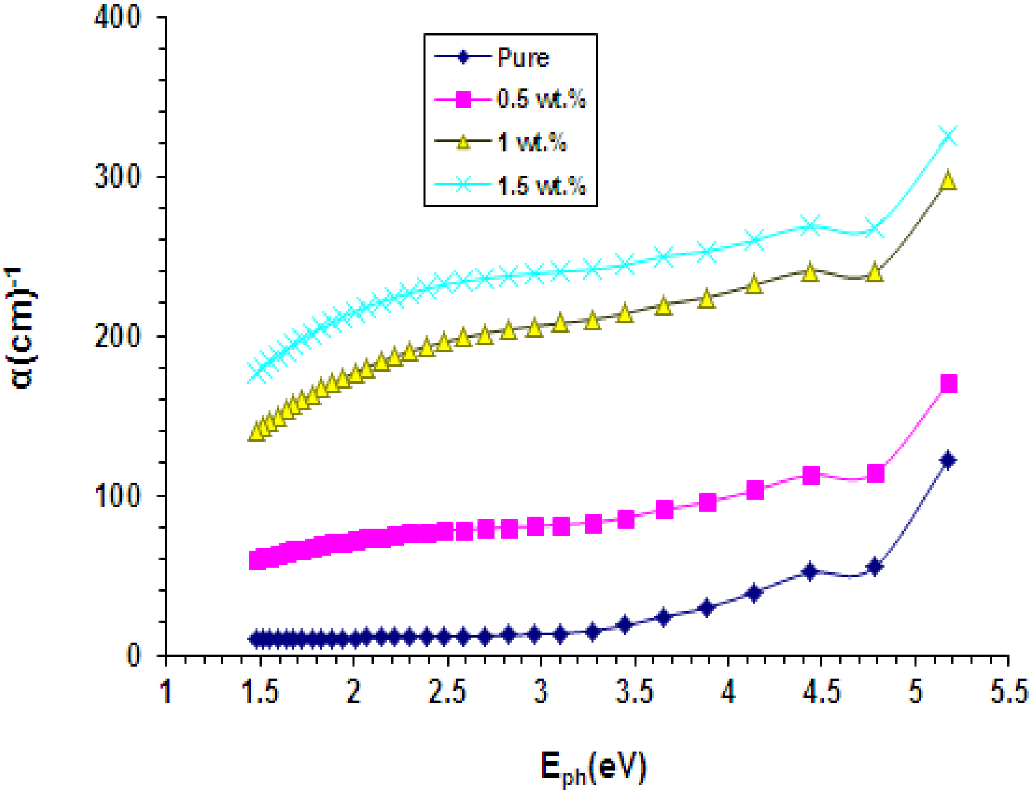


Figure (4-3) Change of absorption coefficient (α) of (PVA-PVP-SiC) nanocomposites with photon energy and different SiC concentrations.

4.4.4Optical energy gap

The values of the allowed and forbidden indirect transissions energy gap was calculated by plotting the graph between $(\alpha hv)^{1/2}$ and $(\alpha hv)^{1/3}$ as a function of the photon energy ((hυ) as shown in Figure (4-4).

$((\alpha hv)^{1/2}=0)$represents the value of the allowed indirect energy gap, where the values of the energy gap were in a state of decreasing with the increase in the rate of doping. This means that the increase in doping led to the displacement of the absorption edge towards lower energies, as the decrease in the energy gap indicates The emergence of new local levels below and above the conduction and valence bands, respectively, within the forbidden gap.

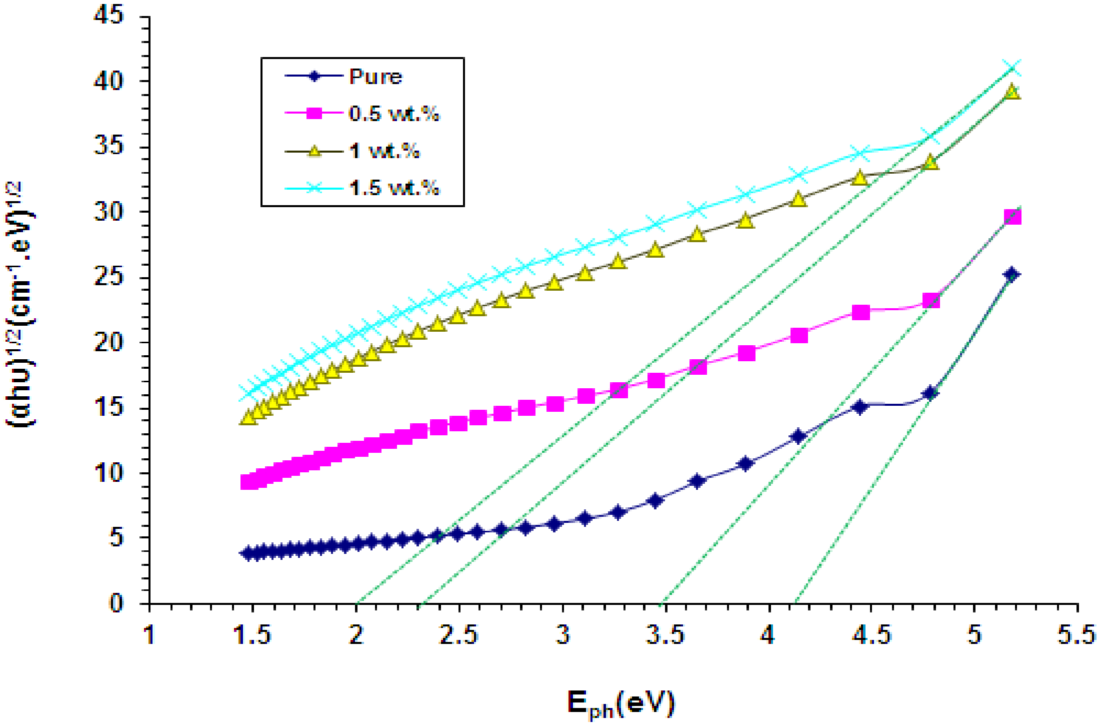


Figure (4-4) The change of$\alpha hv)^{1/2}$ as a function of the incident photon energy of the (PVA-PVP-SiC) complexes.

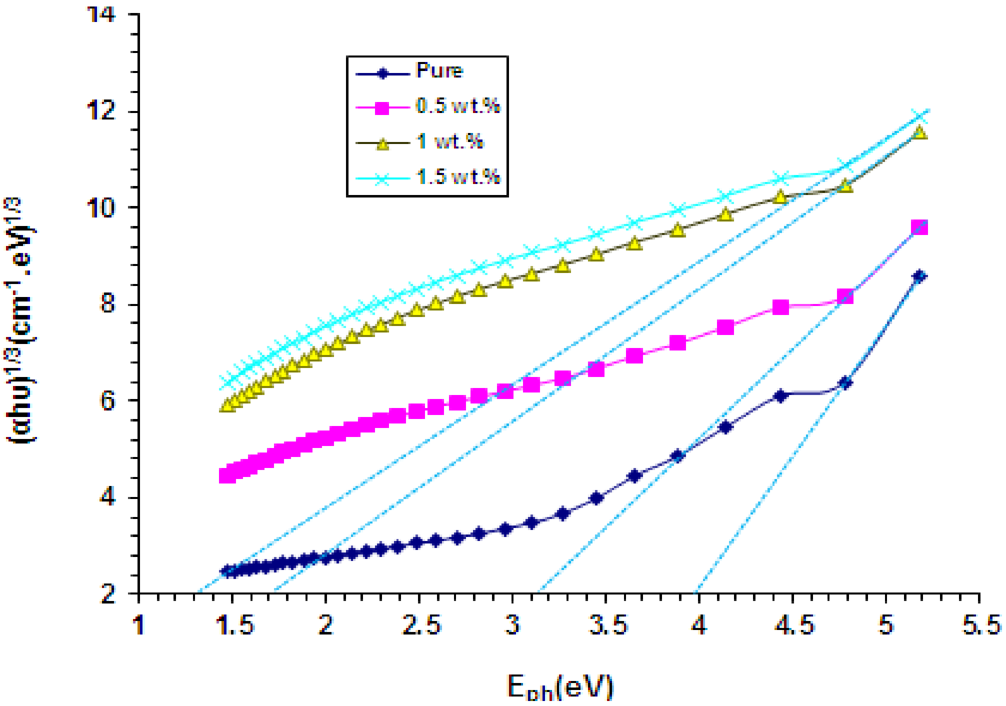
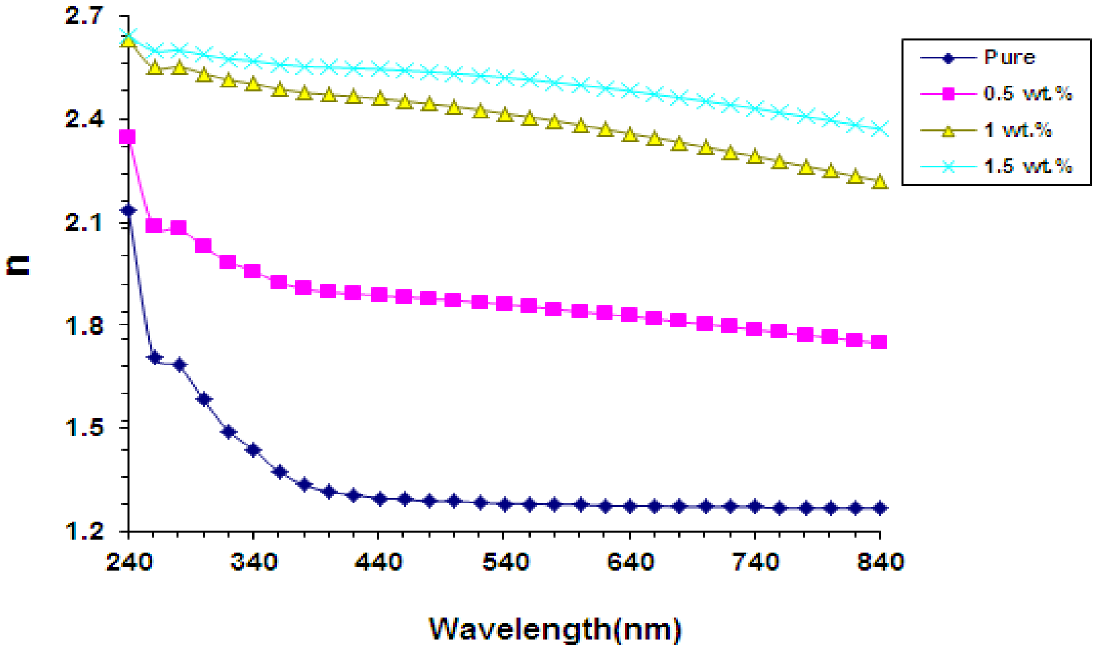


Figure (4.5) Variation of $(\alpha h v)^{1/3}$ for (PVA-PVP-SiC) nanocomposites with photon energy

4.4.5 Refractive Index

The refractive index was found from the relationship (2-16),Figure (4-6)

shows the change in the refractive index of (PVA-PVP-SiC) blend as a function of wavelength, and it can be noticed from this figure an increase in the refractive index with an increase in the concentration of silicon carbide, and the reason for this result is the increase in the density of nanocomposites (that is, as a result of an increase in the number of free electrons). In the ultraviolet region, it can be noticed greater values for the refractive index, due to the low transmittance in this region, but in the visible region, due to the high transmittance in this region**[64].**



Figure(4-6)Change of refractive index (n) of PVA-PVP-SiC nanocomposites with wavelength and different concentrations of SiC Nps.

4.4.6Extinction coefficient

The extinction coefficient (k) of the prepared (PVA-PVP-SiC) nanocomposites was calculated using equation (2-18). Figure (4-7) shows the change of the extinction coefficient with wavelength it can be noticed that the extinction coefficient increases with the increase in the concentration of silicon carbide, and this reason is attributed to the increase in the absorption coefficient with the increase in the concentration of SiC **[65].**

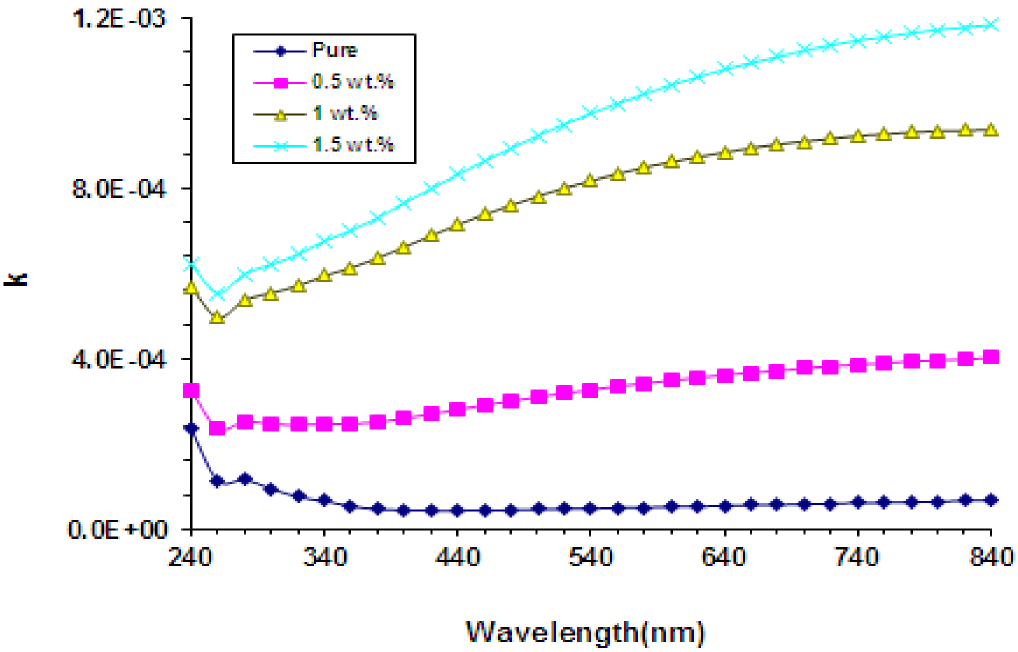


Figure (4-7) The change of the extinction coefficient (k) of the nanocomposites (PVA-PVP-SiC)) with wavelength and different concentrations of SiC.

4.4.7 Real and Imaginary part of Dielectric constant

The dielectric constant for two parts real (ε_1)and imaginary (ε_2)for (PVA-PVP- SiC) nanocomposites are calculated from (2.22) and (2.23) respectively. Figure (4.8) shows the change of (ε_1) as a function of the wavelength. It can be seen that ε_1 considerably depends on (n^2) due to low value of (k^2) so, the real dielectric constant is increased with the increase of the concentrations of (SiC) nanoparticles.

Figure (4.9) shows the change of ε_2 as a function of the wavelength. It can be seen that ε_2 is dependent on values that change with the change of the absorption coefficient due to the relation between (α) and (k). These results agree with the results .**[65].**

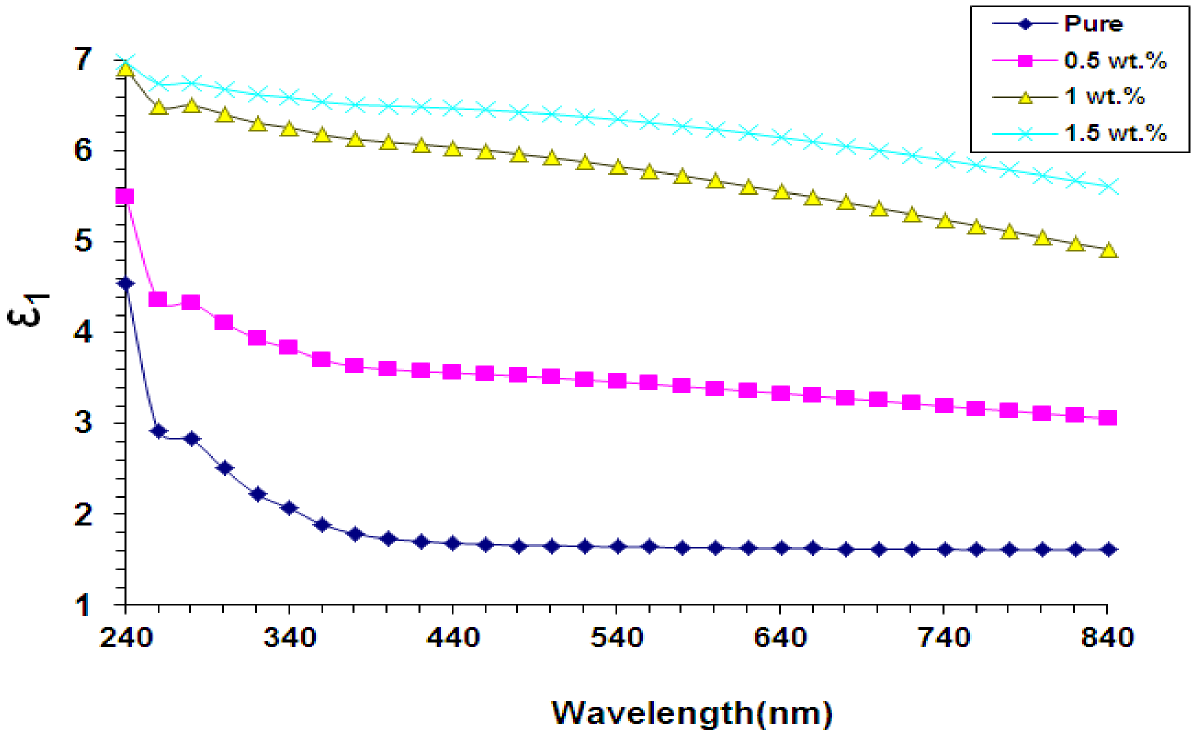


Figure (4-8) Change of the real dielectric constant (ε_1) for PVA-PVP-SIC nanocomposites

With different wavelengths and concentrations of SiC.

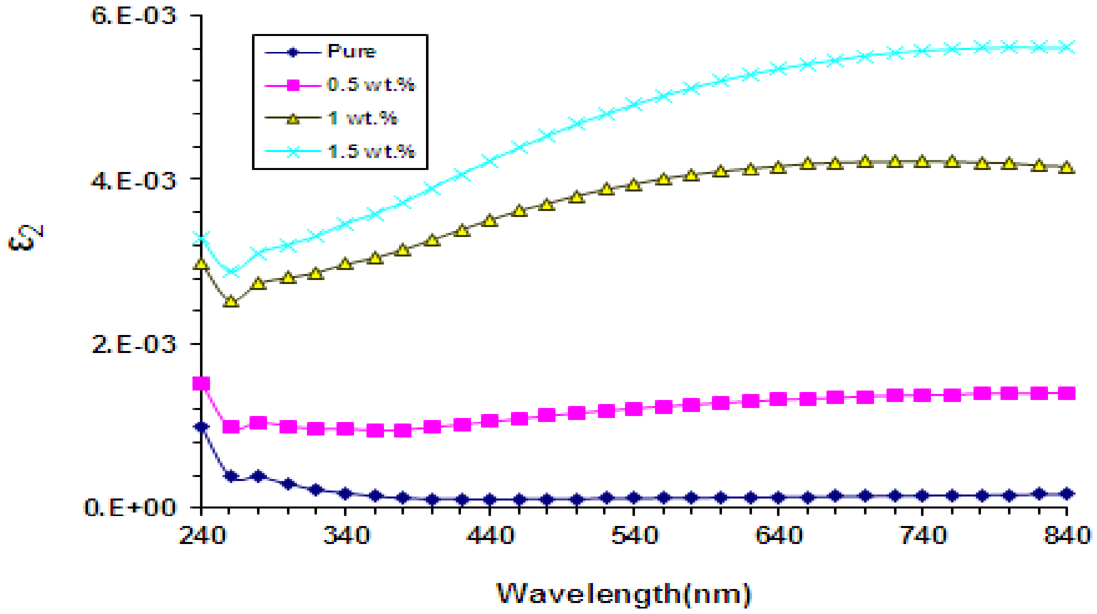


Figure (4-9) dielectric constant($\varepsilon_{2)}$ change for PVA-PVP-SiC nanocomposites With different wavelengths and concentrations of SiC

4.4.8 Optical Conductivity

The optical conductivity values were found from the relationship (2-24). From Figure (4- 10) it can be noticed that the optical conductivity is high in the ultraviolet region and decreases with increasing wavelength and increases with the increase in rang this is due to the increase in the local levels between the valence and conduction bands so the energy gap decreases, which leads to an increase optical conductivity**[66].**

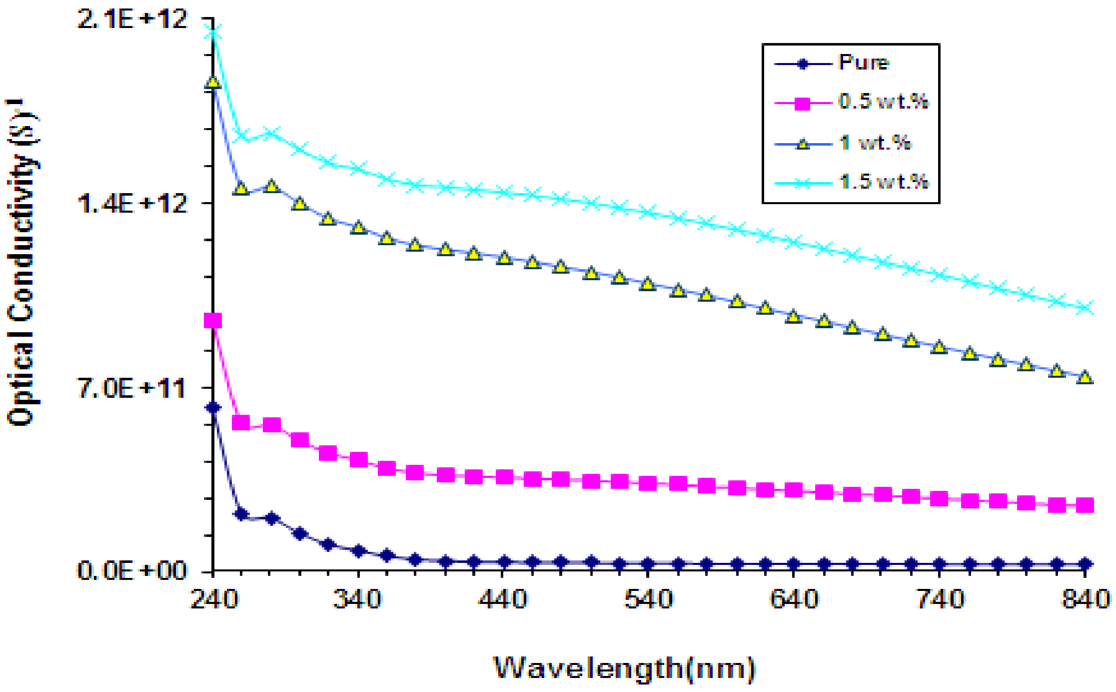


Figure (4-10) The change in the optical conductivity (opσ) of the polymeric complexes (PVA-PVP-SIC)) with wavelength and different concentrations of SIC

Chapter Five

Conclusions
&
Future Work

Conclusions

1-It was found through the study that the adding of silicon carbide nanoparticles to the polymeric blend (PVA-PVP) improved the optical properties .

2-The absorption coefficient is less than ($\alpha > 10^4$ cm) and this indicates that the electronic transitions are indirect for the (PVA-PVP-SiC) nanocomposite

3-The absorbance of (PVA-PVP) blend increases with increasing of SiC (NPS)concentration while transitions decreases with increasing concentration. The absorption coefficient, extinction coefficient, refractive index, real and imaginary dielectric constant of (PVA-PVP) blend increase with increasing concentration of silicon carbide. the optical energy gap decreases with increasing concentration of silicon carbide.

5.2 Future Works

1. The effect of SiC nanoparticles on the thermal conductivity of (PVA-PVP) blend.

2. Study of mechanical properties of (PVA-PVP-SiC) nanocomposites.

3. Study of electrical properties of (PVA-PVP-SiC) nanocomposites.

4. Study of magnetic properties of (PMMA - $Al2O3$) and (PMMA - $ZrO2$) nanocomposites using density functional theory calculations

5.Study of the effect of temperature on the dielectric properties of (PMMA - $Al2O3$ - Ag) and (PMMA - $ZrO2$ - Ag) nanocomposites

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الخلاصة

تم تحضير مركبات النانو البوليمرية لـ (PVA-PVP-SiC) عن طريق إضافة جزيئات كربيد السيليكون النانوية (SiC NPs) بتركيزات وزن مختلفة (0.5 ، 1 و 1.5) بالوزن٪ إلى مزيج كحول البولي فينيل (PVA) والبولي فينيل. البروبيلين (PVP) باستخدام طريقة الصب. كانت الخصائص البصرية لمركبات النانو (PVA-PVP-SIC) بطول موجة (220-820) نانومتر. أظهرت النتائج زيادة الامتصاصية وامتصاص المعامل ومعامل الانقراض ومعامل الانكسار وثوابت العزل والتوصيل البصري لمزيج (PVA-PVP) بينما تقل النفاذية ووفجوة الطاقة بزيادة محتوى SiC NPs. تتميز مركبات النانو (PVA-PVP-SiC) بامتصاص أعلى في منطقة الأشعة فوق البنفسجية. أشارت نتائج الخصائص البصرية إلى أن المركبات النانوية (PVA-PVP-SIC) قد تكون مفيدة في المجالات الضوئية المختلفة.

جمهورية العراق
وزارة التعليم العالي والبحث العلمي
كلية التربية للعلوم الصرفة-جامعة بابل
قسم الفيزياء

دراسات الخصائص البصرية لمتراكبات النانوية (بولي فاينيل الكحول_بولي فاينيل بيروليدون/كاربيد السيلكون)

رسالة مقدمه

إلى مجلس كلية التربية للعلوم الصرفة في جامعة بابل وهي جزء من متطلبات منح درجة الدبلوم العالي التربية\ الفيزياء المواد وتطبيقاتها

من الطالب

هيثم احمد جواد كوير

بكلوريوس تربية فيزياء جامعة بابل2017م

بأشراف

أ.د.احمد هاشم محيسن

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