Republic of Iraq

Ministry of Higher Education

and Scientific Research

University of Babylon

College of Education for Pure Sciences

Department of Physics

Improving the Structural, Optical and Electrical Properties of Nanocarbides Doped Biopolymer for Antibacterial Applications

A Thesis

Submitted to the Council of the College of Education for Pure Sciences, University of Babylon in Partial Fulfillment of Requirements for the Degree of Master in Education / Physics

By

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2022 A.D **1443 A.H**

بِسْمِ اللهِ الرَّحْمنِ الرَّحِيمْ

﴿﴿وَيَسْأَلُونَكَ عَنِ الرُّوحِ قُلِ الرُّوحُ مِنْ أَمْرِ رَبِّي وَمَا أُوتِيتُم مِّنَ الْعِلْمِ إِلاَّ قَلِيلاً﴾﴾

صدق الله العلي العظيم

(سورة الاسراء - الاية ﴿٨٥﴾)

Dedication

To the Great Prophet of Good the Seal of Prophets "Mohammed"

To the owner of the age and time,

"Imam Al-Mahdi"

To my late father and mother

To my brother the martyr (Sallam)

To the best of my life, my children

To my dear wife

To my teacher and brother, Dr. Ahmed Hashem

To all my dear teachers

To everyone who helped me with this work

Wissam ..

ACKNOWLEDGEMENTS

In the name of Allah, the most merciful the most compassionate all praise be to Allah the lord of the worlds and prayers and peace be upon Mohamed his servant and messenger and to his good and pure household. First and foremost, I thank the Almighty Allah for helping and giving me the ability to complete this thesis. Our thanks go to Prophet Mohammed and AhlulBayt (blessings of Allah be upon them all). As I finish my thesis, I cannot but extend my sincere thanks and great gratitude to my dear supervisore Dr. Ahmed Hashim Muhaisin for his distinguished efforts, valuable advice and continuous directions. Many Thanks to the Deanship of the College of Education for Pure Sciences / University of Babylon and the Department of Physics. Finally, I extend my heartfelt thanks to those who supported me and alleviate the difficulties I encountered during my work and to everyone who helped me in one way or another while Working. I wish success to everyone.

WISSAM .. ✍

Supervisor Certification

I certify that the thesis entitled " Improving the Structural ,Optical and Electrical Properties of Nanocarbides Doped Biopolymer for Antibacterial Applications" by " Wissam Obeis Obaid Shehab " has been prepared under my supervision at University of Babylon / College of Education for Pure Sciences as a partial requirement for the degree of Master in Education / Physics.

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Certification of the head of the Department

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

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ABSTRACT

The (PC/SiC-TaC) nanocomposites have been prepared by solution cast method. The effect of (SiC-TaC) nanoparticles concentrations on the structural, optical and electrical properties of (PC/SiC-TaC) nanocomposites have been studied and their applications as antibacterial activity. The experimental results of structural properties for (PC/SiC-TaC) nanocomposites showed the indicated good homogeneity and fine incorporation of (SiC-TaC) nanoparticles in the polymer matrix, the nanoparticles form a continuous network with in the polymer matrix , this network contains nanopaths that allow the passage of charge carriers. The infrared spectrum behavior of polymeric films after adding (SiC-TaC) is agree with its behavior in the polymeric membrane before adding (SiC-TaC) except for some slight changes resulting from the vibration of the bond, this indicates that there is no chemical reaction between the nanocomposite materials but rather aphysical reaction. The experimental results of optical properties for(PC/SiC-TaC) nanocomposites showed that the absorbance, absorption coefficient, extinction coefficient, refractive index, real and imaginary dielectric constants and optical conductivity of (PC/SiC-TaC) nanocomposites were increased with an increase the (SiC-TaC) nanoparticles concentrations. The transmittance and energy band gap were decreased with an increase in (SiC-TaC) nanoparticles concentrations. The (PC/SiC-TaC) nanocomposites have high absorbance in the UV-region. The A.C electrical properties of (PC/SiC-TaC) nanocomposites have been studied in frequency ranging (100 - 5×10^{6}) Hz at room temperature. The experimental results showed that the dielectric constant and dielectric loss of (PC/SiC-TaC) nanocomposites were decreased with an increasing the frequency of applied electric field. A.C electrical conductivity increases with

increasing of frequency. The dielectric constant, dielectric loss and A.C electrical conductivity of (PC/SiC-TaC) nanocomposites were increased with increasing of (SiC-TaC) nanoparticles concentrations. The results of antibacterial applications for (PC/SiC-TaC) nanocomposites which tested against gram-positive (S. aureus) and gram-negative (E. coli) showed that the inhibition zone was increased with increase the concentrations of (SiC-TaC) nanoparticles.

Contents

List of Symbols

Symbol	Description
ε^*	Complex Permittivity
ΔE	Difference in Energy
ε_2	Imaginary Dielectric Constant
A	Area
A.C	Alternating Current
A_o	Absorption
B	Constant Depended on Type of Material
c	Velocity of light
C	Capacitance
C_o	vacuum capacitor
C_p	Electrical Capacitance
d	The Separation between the Plates
D	Dispersion Factor
E	Energy
e	Electron Charge
E. coli	Escherichia Coli
E_{coh}	Cohesive Energy
E_{free}	The Free Atoms sp shell Energy
E_g	Energy Gap
E_g^{opt}	Energy gap between direct transtion
E_o	The Ground-State Energy
E_{ph}	Photon Energy
F	Force
FTIR	Fourier Transform Infrared Radiation
h	Plank constant

H	Electrochemical Hardness
I	The intensity of the transmitted light
I_A	Absorbed Light Intensity
I_o	Incident Intensity of light
IP	Ionization Potential
IR	Infrared Ray
I_T	Intensity of transmittance ray
K	Wave Vector
k	Extinction Coefficient
l	Length
n	Refractive Index
N	Number of Electrons
n*	Complex Refractive
NCs	Nanocomposites
NPs	Nanoparticles
OM	The Optical Microscope
P	Pressure
PC	Polycarbonates
PLA	Polylacticacid
PMMA	Polymethylmethacrylate
PS	Polystyrene
PVA	Polyvinylalcohol
PVAC	Polyvinylacetate
PVP	Polyvinylpyrrolidone
R	Reflectance
r	Exponential constsnt
R_c	Contact Resistance

R_p	Parallel resistance
ε_r	Relative permittivity
S. aureus	Staphylococcus Aureus
SEM	Scanning Electron Microscope
SiC	Silicon Carbide
t	Thickness
T	Transmittance
TaC	Tantalum Carbide
UV	Ultra-Violet
UV-Vis	Ultraviolet-Visible
V_m	Voltage maximum
ω	Angular frequency
α	Absorption Coefficient
ε'	Dielectric Constant
ε''	Dielectric Loss
ε_1	Real Dielectric Constant
ε_o	Permittivity
σ	Optical Conductivity
$\sigma_{A.C}$	Alternating Conductivity
λ	Wavelength
ν	Frequency

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1.1 Introduction

Nanotechnology is one of the most popular topics for current research and development across a wide range of technological fields. This encompasses polymer science and technology and researchs include a wide range of fields[1]. Nanotechnology will enable the development of novel materials providing the basis for the design and development of new properties and structures, which will result in increased performance, reduced cost of maintenance and enhanced functionality[2]. There is a significant feature of nanotechnology, which is the reduction instruments, sensors, and computers, both old and modern, that will have a significant effect on the planet computers of exponentially great strength that generate algorithms to mimic human brains, examples of future miniaturization include biosensors that warn us at the earliest stage of disease initiation, preferably at the molecular level, and medicines that target particular diseases. Nanorobots capable of repairing internal damage and removing toxic pollutants from human bodies, as well as nanoscaled sensors capable of continuously monitoring our local world, are both possibilities. Nanotechnology has a broad variety of possible uses, ranging from nanoscale circuitry and optics to nanobiological structures and nanomedicine. As a result, it necessitates the production of experimental materials as well as multidisciplinary teams of physicists, chemists, and engineers, materials scientists, evolutionary biologists, pharmacologists, and others to cooperate on(i)Nanomaterial synthesis and processing and nanostructures, (ii)A better understanding of the physical properties of the nanometer scale,(iii) Nano-devices or devices that use nanomaterials as building blocks are designed and constructed, work on the fabrication and production of nanomaterials and nanostructures started a long time ago, even before nanotechnology was recognized as a new scientific field, researchs in this field has accelerated rapidly in the last decade, resulting in a flood of literature in a number of journals. Nanotechnology science is increasingly evolving and expanding[3]. In recent years the bulk of polymers were only used in the manufacturing of low-cost,low-functioning goods[4].The polymers can be divided into two denominations: natural and industrial.The natural polymers include proteins, cellulose, starches and rubber, either the industrial include poly(vinyl chloride), nylons polyethylene, polypropylene, polyesters polycarbonate, and polycarbonate, etc[5].

1.2 polymer structure

A polymer consists of organic molecules (macromolecules) of small repeating structural units (monomers) connected to each other by aspecial process of polymerization, and each negative polymer molecule consists of thousands of atoms connected by covalent chemical bonds. Polymer molecules are attracted to each other by forces that depend on the type of polymer[6,7]. Polymers can be classified into two groups according to the effect of temperature on them. They are: (i) thermoplastic polymers : These polymers change their properties depending on the temperature change. When the temperature is increased, they become flexible and viscous; by decreasing the temperature, these polymers return to the original (solid) state. This is because the molecules in the thermoplastic polymer are bound by forces Relatively weak molecular (van der Waals forces) when heated, these molecules can slide over each other as in polystyrene, polyethylene, polypropylene, polyvinyl alcoh[8]. Figure(1.1) shows the atomic configuration of thermoplastic polymer.

Figure (1.1). Atomic configuration of thermoplastic polymers[8].

(ii) Thermoset polymers: which are changing chemically when heated. Thermoset materials are usually three-dimensional lattice polymers in which there is a high degree of cross-linking between the polymer chains. After being heated, these polymers become insoluble, non-conductive, and hard because the molecules of these polymers are connected by strong covalent chemical bonds. Phenol-formaldehyde resin and urea-formaldehyde resin are examples of this type of polymer [6,9,10,11]. Figure(1.2) shows the atomic configuration of thermosetting polymers.

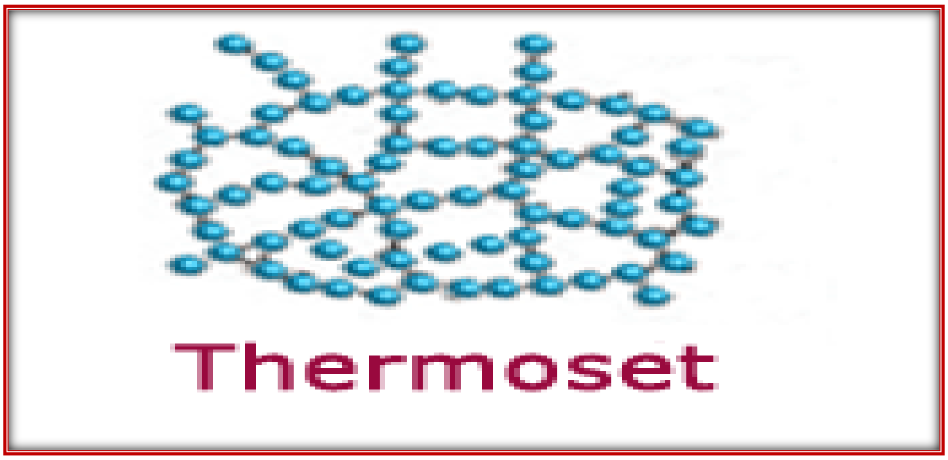


Figure (1.2). Atomic configuration of thermosetting Polymers[8].

Materials that have a polymer matrix with a conductive filler are known as conductive polymer composites[12,13]. These compounds are known for their high dielectric constants and for being highly conductive. This is achieved by conductive padding that forms a mesh throughout the compound allowing current to flow through the compound. The conductivity of these compounds can increase by several orders of magnitude. Since the matrix is composed of a polymer, these compounds have the potential to increase flexibility, if the polymer used in the matrix is flexible. The compound can be brittle and weak due to the amount of filler needed to produce a highly conductive material. The main advantage of conductive polymer composites is that they display the properties of both metal and polymer[13,14]. Conductive polymer compounds can consist of two types of microstructures. A system can contain either a random microstructure or a discrete microstructure. The random microstructure consists of a polymer matrix with filler particles placed intermittently throughout the matrix. These compounds have isotropic properties and the filler does not show any bias to its location. The separate microstructure consists of filler particles showing a bias for their location. These compounds contain filler-rich regions along with polymer-rich regions[13,16]. Figure (1.3) shows a cartoon of a discrete microstructure versus a random microstructure .

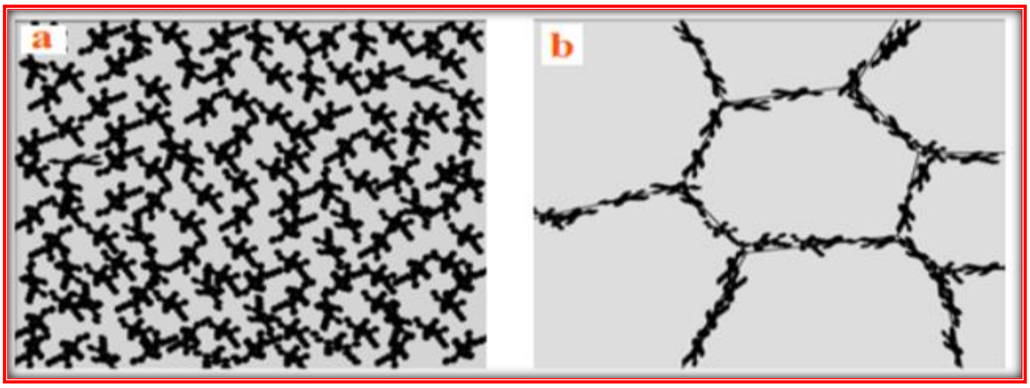


Figure (1.3). a cartoon of a discrete microstructure versus a random microstructure[15].

1.3 Nanocomposites

Nanocomposites consist of polymers that may be natural or synthetic, and they are nanomaterials, which refer to materials with nano-sized topography or composed of nano-sized building components[16]. Although the terms nanomaterials and nanocomposite represent new and exciting areas in materials science, they have been used for centuries when they exist in nature. However, methods for characterizing and controlling the structure at the nanoscale have only stimulated much later[17].A nanocomposite, is a conventional compound consisting of two parts, a filler and a matrix. In a conventional composite usually a fiber such as glass fiber or carbon fiber is used as a filler, in a nanocomposite, the filler is a nanomaterial. Examples of nanomaterials are carbon nanotubes, carbon fiber tubs, and nanoparticles such as gold, diamond, silver, silicon and copper[18].The dispersion of inorganic nanocomposites into an organic polymer to form polymer nanocomposites has gained increasing attention in recent years. The fundamental and important role that nanostructure control composition and morphology play in their applications, The new properties of nanocomposites can be obtained through the successful transfer of the properties of the original components into a single materials [19].An important and significant challenge in developing nanocomposites is to find ways to create macroscopic components that take advantage of the unique physical and mechanical properties of the very small objects within them. On the other hand, the fracture toughness of such biocomposites depends on the ultimate tensile strength(T) of the reinforcement. Crucially the use of nanomaterials allows the maximum theoretical strength of the material to be reached, because the mechanical properties become increasingly insensitive to defects at the nanoscale[20]. Electrical, thermal and electronic properties and the electrochemical properties of nanocomposites can differ significantly from those of their constituent[21]. The basic theory of nanocomposites is based on the principle that there is a very wide interface between the nano-sized building blocks and the polymer matrix that our study is based on this method or the nanocomposite[22].

1.4 Applications of Polymer Nanocomposites

The applications of polymer nanocomposites are based on: the matrix and the nanocomposites[23]. Among its many applications are:

- Cars (gasoline tanks, fenders, interior and exterior panels...etc).
- Construction (pull out the shape, panels).
- Electronics and electricity (printed circuits and electrical components).
- Food packaging (packaging, films).
- Cosmetics (controlled release of active ingredients).
- Dentistry (filling materials).
- Environment (biodegradable materials).
- Gas barrier (tennis balls, food and beverage packaging).
- Flame retardants, military, aerospace and commercial applications.

It can be noted that there are many industrial and medical applications of nanomaterials related to many fields, including engineering, biology, chemistry, computing, materials science, military applications, and communications, but their effects are difficult to enumerate benefits of nanotechnology include improved manufacturing methods, water purification systems, improved food production methods and energy networks, physical health promotion, nanomedicine. Products made with nanotechnology may require little labor earth, or maintenance, are high in productivity, low in cost, and have modest material and energy requirements[24].

1.5 Carbides

In chemistry, carbide is a compound composed of carbon and a less electronegative element. Carbides can be generally classified by the type of chemical bonds as follow[25].

a. The salt (ionic bonds) .

b. Interstitial compounds.

c. Covalent compounds.

d. Transition metal carbide.

Examples include calcium carbide, tungsten carbide, silicon carbide and tantalum carbide. The silicon carbide is hard material "covalent carbide" and industrially important[25].

1.6 Tantalum Carbide (TaC)

Tantalum carbide (TaC) is a ceramic material that has the ability to withstand very high temperatures. It is also used industrially in the manufacture of cutting tools because of its hardness that exceeds that of diamond [26]. It can also be added to the crystal structure of tungsten carbide alloy. The tantalum carbide (TaC) nanomaterial is strikingly interesting, because it contains some characteristics such as high hardness, high melting point max (3880^{o}C)[27]. This material is considered resistant to chemical attack and oxidation, and has good and excellent catalytic and thermal properties and limits of electronic conductivity[28,29]. The chemical properties of this substance are attributed to the mixed metal covalent bond [30]. One of the main uses of TaC is as phase hardening in composites to increase strength and wear resistance [31]. Tantalum carbide (TaC) is difficult to produce by sintering to a high melting point of (3880°C).TaC is difficult to sinter in conventional or hot pressing furnaces. Furnaces designed for these higher temperatures are usually very expensive[32]. Tantalum carbide has good physical properties as shown in (1-1) Table

Table (1-1). physical properties of Tantalum Carbide

Properties	Tantalum Carbide
Melting point	3,880 C°
Density	14.3g/cm^3
Molar mass	192.96g/mol
Chemical formula	TaC
Appearance	Brown-gray powder
Boiling point	(5,470–4,780) C°
Solubility	Soluble in ($CHCl_3$) and HF-HNO_3 mixture

1.7 Polycarbonates(PC)

Polycarbonates (PC) are a group of thermoplastic polymers that contain aggregates of carbonates in their chemical structures. They are strong, rigid, and sometimes optically transparent materials. Polycarbonate is easily fabricated and thermoformed. Because of these properties, polycarbonate finds in many applications . Polycarbonates got their name because they are polymers containing carbonate groups abalance of beneficial features, including temperature resistance, shock resistance, and optical properties, places polycarbonate between commodity plastics and engineering plastics[33].

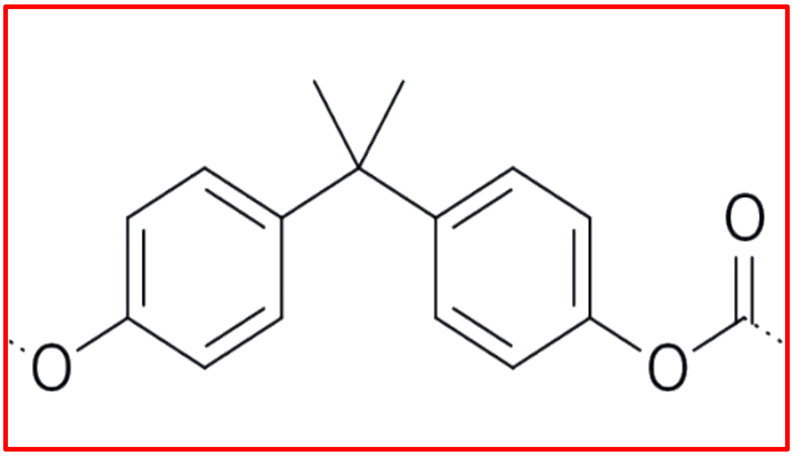


Figure (1.4). chemical structure unit of Polycarbonate[33]**.**

Polycarbonate is mainly used in electronic applications that take advantage of security features. Being a good electrical insulator with heat-resistant and flame-retardant properties, it is used in many products associated with telecommunication devices and electrical appliances and can also act as an electrical insulation in highly stable capacitors [34].

1.8 Silicon Carbide (SiC)

Silicon carbide is also known as carborundum and is found in nature in the form of the extremely rare mineral Moissante. Silicon carbide is a compound of silicon and carbon with the chemical formula (SiC). Silicon carbide powder has been produced since 1893 for use as abrasives. Granules of silicon carbide can be bonded together by roasting to form very hard ceramics, so it is widely used in applications that require high tolerances, such as automobile brakes, ceramic plates, in bulletproof vests, high speed steel polishing processes, deep drawing dies and carbide inserts[35].

Table (1-2). physical properties of silicon carbide[35].

Properties	Silicon Carbide SiC
Density	3.21 g/cm3
Melting Point	2730 C0
Thermal Conductivity	3.6 W/cm.K
Crystal Structure	Cubic,cF8
Lattice Constant	4.3596 Å
Grain Size	75 µm

SiC particles in the particles may behave as abrasives at the interface of the work piece during machining and affect the mechanical properties of the composites i.e. hardness and tensile strength the silicon carbide material in the work piece plays an important role in it as machinability, so it represents abrasive areas in the metal that cause excessive wear of the tool, increases the cutting force, and has a significant impact on the quality of the machined surface[36]. Silicon carbide has good physical properties as shown in (1-2) Table [35].

1.9 Literature Survey

K. Shameli *et. Al*, in 2010 [37], study the Silver/poly (lactic acid) nanocomposites: preparation, characterization, and antibacterial activity.The results indicated that silver /PLA-NC films have strong antibacterial activity with the increase in the concentration of Ag-NPs in the PLA.

In (2011), **K. Sivaiah *et al*,** [38], study the electrical and optical properties of (PVP- Li) and (PVP- Ag) polymer films. They found the electrical properties and dielectric constant of these films showing a decreasing trend and an increase in the frequency. The energy gap decreases with the increase of the Li, Ag concentration while the absorption increases with the increase of the concentration of nanoparticle.

B. Hussein and A Hashim, in (2012)[39], study the electrical dielectric properties of (PS-$BaSO_4.5H_2O$) composites. They found that the dielectric constant decreases with increasing frequency and increase with increasing of the ($BaSO_4.5H_2O$) content. The dielectric loss decreases with increasing of the frequency and increasing of the ($BaSO_4.5H_2O$) content by weigh. The electrical conductivity increases with the increase in the frequency and ($BaSO_4.5H_2O$) wt%.

In (2013)**S. Devikala, *et al*,** [40], study the electrical properties of (PMMA-ZrO_2).They found that the electrical conductivity of the composites increases with increasing (ZrO_2) concentrations, the dielectric loss, and the dielectric constant decreases with increasing frequency.

W. K. Kadhem , and Habeeb, in (2014)[41], study the optical properties of (PVA-PVAC-Ti) nanocomposites where the nanocomposite was prepared using the casting method with different weight ratios of nano-titanium. They found that the absorbance increases with increasing concentration of titanium particles. But the transmittance decreases with increasing concentration, the electronic transitions are indirect, while the optical constants increase with increasing concentration.

In (2015) **S. Sujumaran, *et al*,**[42], study the characterization of the (PVA-Al_2O_3) composite thin films prepared by the dipping method. They found that dependence of temperature and frequency for dielectric properties. The results also showed the study of insulating properties. The results indicated a higher refractive index, dielectric constant and lower dielectric loss for (PVA-Al_2O_3).

In(2016)**J. J. Mathen, *et al*,**[43], study the improve of the optical and dielectric properties of PVA matrix with nano-ZnSe. The results showed that the dielectric constant and loss dielectric increase with increasing of ZnSe nanoparticles concentration. The optical conductivity increases with increasing the nanoparticles concentration.

A. Goswami, *et al.*in (2017)[44]**,** study carboxymethylcellulose (CMC) and (PVA) thin films by solution casting. Vanadium pentagonal oxide was prepared for the production of bio-nanocomposites (CMC/PVA-V_2O_5) by in situ precipitation. The electrical conductivity of alternating current was measured at different frequencies. It was found that the conductivity rises at a higher frequency, and the bandgap decreases at UV-VIS spectra. The nanocomposites appear to have a strong electrical behavior.

In (2018)**B. Gurswamy, *et al***,[45], study The doping of SnO_2 nanoparticles on the structural, optical, electrical and thermal properties of the polymer blend (PVA-PVP). Membranes of the nanocomposites (PVA-PVP-SnO_2) were prepared using the solution casting technique. An infrared Fourier transform study showed that SnO_2 nanoparticles react with the (OH) group of (PVA) and the carboxyl group (PVP) to form the compound within the mixing matrix. The optical study showed increased absorption in the UV region and transparency in the visible region.

A. Hashim, *et al.*, in (2019) [46], study structural and optical properties for nanocomposites of polyvinyl alcohol (PVA)–polyethylene oxide

(PEO)–copper oxide (CuO). They found that the absorbance of the (PVA–PEO) blend rises as the concentration of CuO nanoparticles rises. As the concentration of CuO nanoparticles increases the transmittance decrease.

Q. Jebur, *et al.* in(2020)[47], study the structural and dielectric properties of (PVA-PEO-Fe_2O_3) nanocomposites.The results showed that the dielectric constant and dielectric loss are decreased while the electrical conductivity increases with the increase in frequency of applied electric field. The absorbance of (PVA-PEO-Fe_2O_3) nanocomposites improved as concentrations of iron oxide nanoparticles increased.

in (2021) A. A. Abid, *et al*.[48], study the polymer mixture (PVA-PVP)-Carbon black (C.B N_{375}) nanocomposites.by casting procedure . and they studied the optical microscope, FTIR, and optical ,electrical properties. They found that The absorbance of(PVA-PVP-C.B)nanocomposites increased with growing concentrations of carbon black (C.B) nanoparticlse .The electrical conductivity (A.C), dielectric loss and dielectric constant of all the samples were increased with increasing of the nanoparticlse concentrations.

1.10 The Aims of work

The aims of this work are:

1. Preparetion of PC/SiC-TaC nanocomposites to use in medical applications.

2. Studing the structural , dielectric and optical properties of PC/SiC-TaC nanocomposites.

3. Test antibacteral application of PC-SiC/TaC nanocomposites .

2.1 Introduction

This chapter includes a theoretical description (the theoretical part). It focuses on theories of optical properties, absorption, polarization and electrical properties in particular. There is increasing research in nanocomposites due to improvements in optical and electrical properties in particular. Nanoparticles represent advanced technological materials due to their properties attractive electronics and its high refractive index.

2.2 The Structural Properties

2.2.1 The Optical Microscope(OM)

The Optical Microscope(OM) measures good homogeneity and fine incorporation of nanoparticles in the polymer matrix. The nanoparticles form a continuous network with in the polymer matrix , this network contains nanopaths that allow the passage of charge carriers.

2.2.2 Scanning Electron Microscope(SEM)

(SEM) (Scanning Electron Microscope) is a type of electron microscope that produces images of a sample by scanning the surface of the sample with a focused beam of electrons. Electrons interact with atoms of the sample containing information about the nature of the surface topography in the sample. (SEM) can detect secondary electrons emitted by atoms excited by the electron beam depending on the topography of the sample[49].

2.2.3 Fourier Transform Infrared Radiation (FTIR)

FTIR (Fourier Transform Infrared) is a technique useful for obtaining the infrared spectrum of absorption or emission of a substance in its solid, liquid or gaseous state. The (FTIR) spectrometer collects high-resolution data at the same time over a wide spectral range. This confers a significant advantage over dispersion spectrophotometers, which simultaneously measure intensity over a specified range of wavelengths. The (IR) Fourier transform came from the fact that the Fourier transform (acomputational process) converts the raw data into the actual spectrum[50].

2.3 The Optical Properties

Studies and research on the optical properties of many compounds have increased due to their applications in optics such as optical information, optical modulation, and optical data storage. The study of optical absorption is useful in determining direct and indirect transitions and elucidating the electronic structure[51]. When add nanoparticles into the polymer, the electrical, optical and structural properties of the materials will be improved. Polymer nanoparticles have been studied as alternative materials for optical applications such as micro-optical elements and planar waveguide devices. Developments in the structures of polymer nanocomposites are due to the ease of processing and production, light weight, good adhesion to reinforcing elements and resistance to the corrosive environment [50,51].

2.3.1 The Absorbance (A_o) and Transmittance (T)

To study the optical properties of polymers has multiple applications such as optical devices, electronic devices such as solar cells, fuel cells, solid state batteries and medical technological applications[52].

If I_o is the intensity of the incident light and I is the intensity of the transmitted light

$$I=I_o\, e^{-\alpha d} \qquad (2 - 1)$$

Where (α) is the absorption coefficient and(d)is the path length of the absorbing species.

The absorption coefficient α can be calculated from the absorption data as[53,54].

$$\alpha = 2.303 \frac{A^{o}}{d} \qquad (2-2)$$

for higher photon energies, the simplified general equation is

$$\alpha h\nu = B\,(h\nu - E_g^{op})^n \qquad (2-3)$$

Where $(h\nu)$ is the energy of absorbed radiation ,(n) is the parameter connected with distribution of the density of stales and *(B)* is the proportionality factor. The index n=1/2 for allow direct transition and (n = 2) for indirect transition energy gaps [55,56] Thus from the straight-line plots of $(\alpha h\nu)^2$ versus hν and $(\alpha h\nu)^{1/2}$ versus hν the direct and indirect energy gaps of insulators dielectrics can be determined. The Beer-Lambert law has implicit assumptions that must be met experimentally for it to apply otherwise there is a possibility of deviations from the law to be observed[55]. The reflectance (R) has been determined from values of transmission (T) and absorbance (A_o) , using the relationship[56].

$$A_o+R+T=1 \qquad (2-4)$$

2.3.2 The Absorption Regions

The absorption regions are three regions [57].

(A) High absorption region: the magnitude of absorption coefficient (α) is larger or equal to (10^4 cm^{-1}) .

(B) Exponential region: the value of absorption coefficient (α) is

($1\ cm^{-1} < \alpha < 10^4\ cm^{-1}$) .

(C) Low absorption region: the absorption coefficient (α) is very small, ($\alpha < 1 cm^{-1}$), as shown in figure (2.1) which shows the absorption regions.

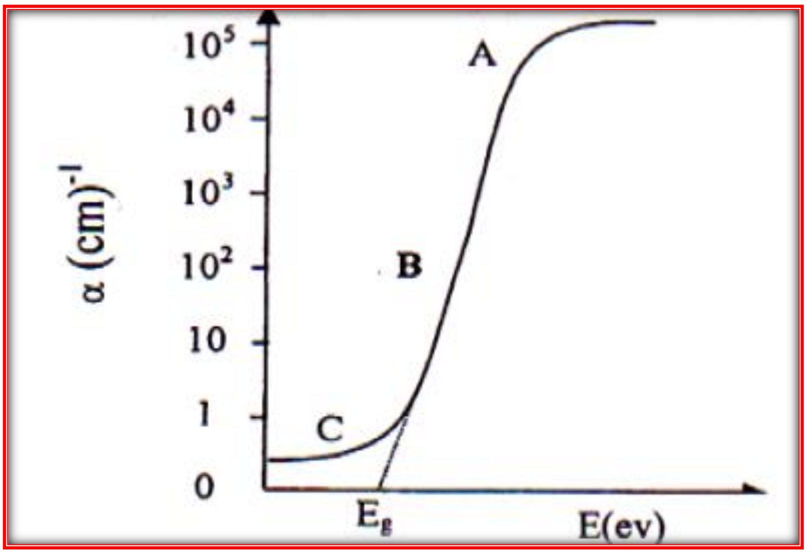


Figure (2.1). The absorption regions

2.3.3 The Refractive Index and Extinction Coefficient

The refractive index of a substance is defined as the ratio of the value of the speed of light in a vacuum to the speed of light in the sample[58].

$$n = \frac{c}{V} \qquad (2 - 5)$$

where (c) the velocity of the light in vacuum and (v) the velocity of the light in specimen .

$$n^{*} = n - ik \qquad (2 – 6)$$

Where: (n *) is a complex refractive index, (n) is a real part of the refractive index and (k) is an imaginary part of the refractive index or called (the extinction index).

The relationship between the absorption coefficient and molar absorbance or extinction coefficient (k) is given by law.

$$k = \frac{\alpha\lambda}{4\pi} \qquad (2 – 7)$$

where (λ) the wavelength

The real part of the refractive index (n) can be calculated by the following relationship

$$n = \frac{1+\sqrt{R}}{1-\sqrt{R}} \qquad (2-8)$$

Where (R) is the reflectanc.

2.3.4 The Dielectric Constant and Optical Conductivity

The complex permittivity explains the relationship between the electric field and the magnetic field in a material. The imaginary part is directly related to the resistance, while the real part shows us whether the material has an capacitive or inductive optical response. The real part and the imaginary part were obtained from the dielectric constant using the relationship[59].

$$\varepsilon_1 = (n^2 - k^2) \qquad (2-9)$$

$$\varepsilon = \varepsilon_1 - i\varepsilon_2 \qquad (2-10)$$

$$\varepsilon_2 = 2nk \qquad (2-11)$$

The optical conductivity is determined by the relationship :

$$\sigma = \frac{\alpha n c}{4\pi} \qquad (2-12)$$

2.4 The Electrical Polarization

If an external electric field affects the terminals of a capacitor consisting of an electrical insulator between its plates, the local displacement of the centers of positive and negative charges will occur, and induced dipole moments will be generated, i.e. an electric polarity process occurs. Its value is equal to the sum of the moments of all the dipoles present in the sample unit volume[60]. The polarization value equals to the sum of moments of all dipoles existed in the material unit volume .

$$m = a E_i^{-} \qquad (2\text{-}13)$$

Where : m = electrical dipole moment, a = polarity of an atom or a molecule and E_i^{-} = internal field of a molecule. The total dipole moment(P) for a unit volume is[61].

$$\vec{p} = N_v m \qquad (2-14)$$

Where: N_v = number of molecules for a unit of volume. The increase in the charge density (σ + P) leads to an increase in the flux density (D_e), which can be defined as[62].

$$\vec{D}_e = \varepsilon_o \vec{E} + \vec{P} \qquad (2\text{-}15)$$

There are a number of possibilities for polarization to occur, including :

- Electronic polarization: when an external electric field is applied, the positively charged nucleus will move in one direction and the negatively charged electron cloud will be deformed in another direction in the atom, resulting in a dipole.

- Ionic polarization: when a substance that has positive and negative ions placed inside an external electric field, the ions will be displaced according to the direction of that field, resulting in local dipole moments.

- Polarization dipole: when a material with permanent dipoles placed inside an external electric field, then these permanent dipoles of the material will arrange to align with the direction of the field, creating a net polarization[62].

2.5 The A.C Electrical Properties

To store electrical energy, insulators can be used by charge separation when the electron distributions around the constituent atoms or molecules are polarized by an external electric field. The complex permittivity of the material can be expressed in[61].

$$\varepsilon^{*} = \varepsilon_a - i\varepsilon_b \qquad (2\text{-}16)$$

where ε_a and ε_b are the real and imaginary terms of the complex permittivity and i = $\sqrt{-1}$. The real term of the permittivity can be defined as[62].

$$\varepsilon_a = \varepsilon_0 \bar{\varepsilon} \qquad (2\text{-}17)$$

The magnitudes of (ε_a) and (ε_b) depend on the frequency(ω) of the applied electric field. The magnitude of (ε_a)or the dielectric constant ($\bar{\varepsilon}$) indicates the ability of the material to store energy from the applied electric field[63]. The capacitance of a capacitor consisting of two parallel plates we can get from [64].

$$C = \bar{\varepsilon}\, \varepsilon_o \frac{A}{t} \qquad (2\text{-}18)$$

Where:(έ) is a dielectric constant , (t) is the sample thickness and (ε_o) vacuum permittivity. The following relationship can be applied to calculate the value of the dielectric constant [65].

$$\bar{\varepsilon} = \frac{C_p}{C_o} \qquad (2\text{-}19)$$

Where: (C_o) vacuum capacitance ,(C_p) parallel capacitance. The dielectric loss (ε″) is given by[66].

$$\varepsilon'' = \bar{\varepsilon} D \qquad (2\text{-}20)$$

Where (D) is known as the dispersion factor. It measures the electrical energy lost in the sample from the applied field and it will be converted into thermal energy in the sample. The power dissipated in the insulator can be determined by the presence of the alternating voltage as a function of the(AC) conductivity by[66].

$$\sigma_{A.C} = \omega\, \varepsilon''\, \varepsilon_0 \qquad (2\text{-}21)$$

where(ω)is angular frequency , $\omega = 2\pi f$

2.6 Antibacterial applications

Antibiotics often lose their effectiveness over time due to the emergence and spread of drug resistance by bacterial pathogens, which leads to the generation of the so-called “antibiotic resistance crisis” and infections in addition to the huge amounts of medical costs that may reach billions of dollars annually[67,68].Particles and nanomaterials have become the global platform for many therapeutic applications because of the unique physical and chemical properties of these materials and provide treatment for drug-resistant bacteria [69,70].The antibacterial activity of multiple nanomaterials is expected to play an important and alternative role for other antibacterial agents[70]. The important and unique properties of some nanomaterials such as changing their size or shape, surface properties, optical properties, low cell toxicity, and high stability make them attractive in many fields of medicine[71] .Because of those qualities and properties that characterize some of these nanomaterials, they have anti-fungal and anti-bacterial activity, so nanomaterials can be combined with other certain biological materials to transfer anti-bacterial properties to the material, thus improving the value of that material and its applications[72].The nanoparticles are attached to the antibacterial drugs via covalent or non-covalent bonds whereby the antibacterial drugs reach the site of action effectively[73]. When bacteria are active in the affected sites in the body, whether on the skin or in the intestines, the rates of secretion of their output and waste naturally increase, which increases the acidity of the medium in it; It drops below 5 degrees, and the more you activate the degree more, and therefore this medium is ideal for changing the charge of the nanocomposite from negative to positive, only when the body has a bacterial infection, and this is what is required, and then attraction occurs between the nanocomposite and the cell membrane of bacteria cells to eliminate therefore. This process also ensures that the compound is not attracted to healthy cells, as long as there are no bacteria in the medium, which makes it biologically safe[73].

3.1 Introduction

This chapter includes the stages of samples preparation for (PC/SiC-TaC) nanocomposite, sample tests and measurements stages, including: optical microscopy, FTIR, SEM, optical measurements, A.C electrical properties measurements and measurements of antibacterial activity.

3.2 The Materials Used in This Work:

1- Polycarbonate(PC): the polymer is used as powder . Manufacture: Teijin Human Chemistry - Japan company.

2- Tantalum Carbide(TaC): used as powder (1µm,cubic) and high purity (99%) from EPRUI company.

3- 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 (PC/SiC-TaC) Nanocomposites

The nanocomposite (PC/ SiC-TaC) was prepared through the :

(1g) of the polymeric material (polycarbonate) (PC) was dissolved in (30) ml of chloroform alcohol and a magnetic stirrer was used to mix the material and obtain complete dissolution of the solution. The SiC and TaC nanoparticles are added each one to polymer with different concentrations which are (1.2, 2.4, 3.6 and 4.8) wt.%. The casting method is used to prepare the samples of (PC/ SiC-TaC) nanocomposites in the template (petri dish has diameter 10 cm)and left to dry for two days.

Figure (3.1). Magnetic stirrer used in the work

3.4 Measurements of Structural Properties ForNocomposites

3.4.1 Microscopic Examination

Samples (PC/SiC-TaC) are examined using an optical microscope (Olympus (ToupView) type (Nikon-73346)) with magnification (x10),in the College of Education for Pure Sciences, University of Babylon.

Figure (3.2). Optical Microscope used in the work.

3.4.2 Fourier Transform Infrared Spectrometer (FTIR)

FTIR spectra of (PC/SiC-TaC) were recorded by FTIR (Brucker Company), German origin, type vertex-70) Fourier transform infrared spectrometer in the wavelength range (500-4000) cm^{-1}, in the College of Education for Pure Sciences, University of Babylon.

Figure (3.3) Fourier transform infrared spectroscopy device used in the work.

3.4.3 Scanning Electron Microscope (SEM)

The surface morphology of (PC/SiC-TaC) nanocomposites were for the concentration (1.2, 2.4, 3.6 and 4.8) wt.%. Were tested using a scanning electron microscope (Zeiss, Sigma, German origin) at Shahrud University of Technology, Iran.

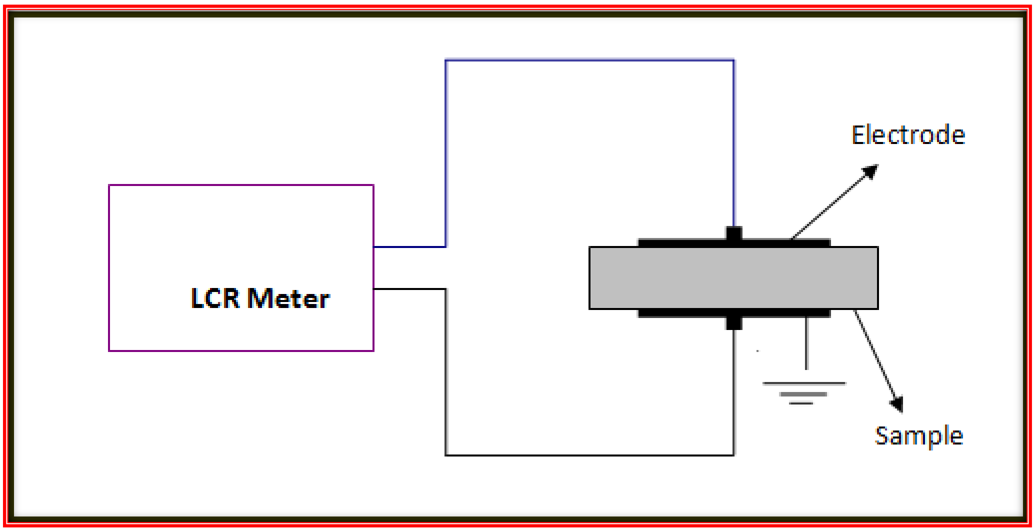
3.5 Optical properties measurements

The absorption spectrum of (PC/SiC - TaC) nanocomposites with a thickness of (100µm) in the wavelength range (280-880)nm was recorded using a spectrophotometer(Shimadzu, UV-1800A°) as shown in figure (3.4).The absorption spectrum was recorded at room temperature.

Figure (3.4): The photographic of spectrophotometer

3.6 Measurements of A.C Electrical Properties For Nanocomposites

The A.C electrical properties of (PC/SiC-TaC) nanocomposites are measured by measuring the capacitance (C_p) and dispersal factor (D) using a type LCR meter (HIOKI 3532-50 LCR HI TESTER) using different frequencies of (10^2 Hz –5MHZ) at room temperature as shown in figure (3.5), in the College of Education for Pure Sciences, University of Babylon.



Figure(3.5). Schematic diagram for A.C electrical properties measurement

3.7 Antibacterial Activity Application Measurements of Nanocomposites

The antibacterial activity of (PC/SiC-TaC) nanocomposites samples was tested by diffusion method. Antibacterial activities were carried out using Gram-positive (Staphylococcus aureus) and Gram-negative (Escherichia coli) organisms. Bacteria (Staphylococcus aureus and Escherichia coli) were cultured in Muller-Hinton Medium. Discs (PC/SiC-TaC) were placed on media and incubated at (37°C) for 24 hours. The diameter of the damping zone was measured.

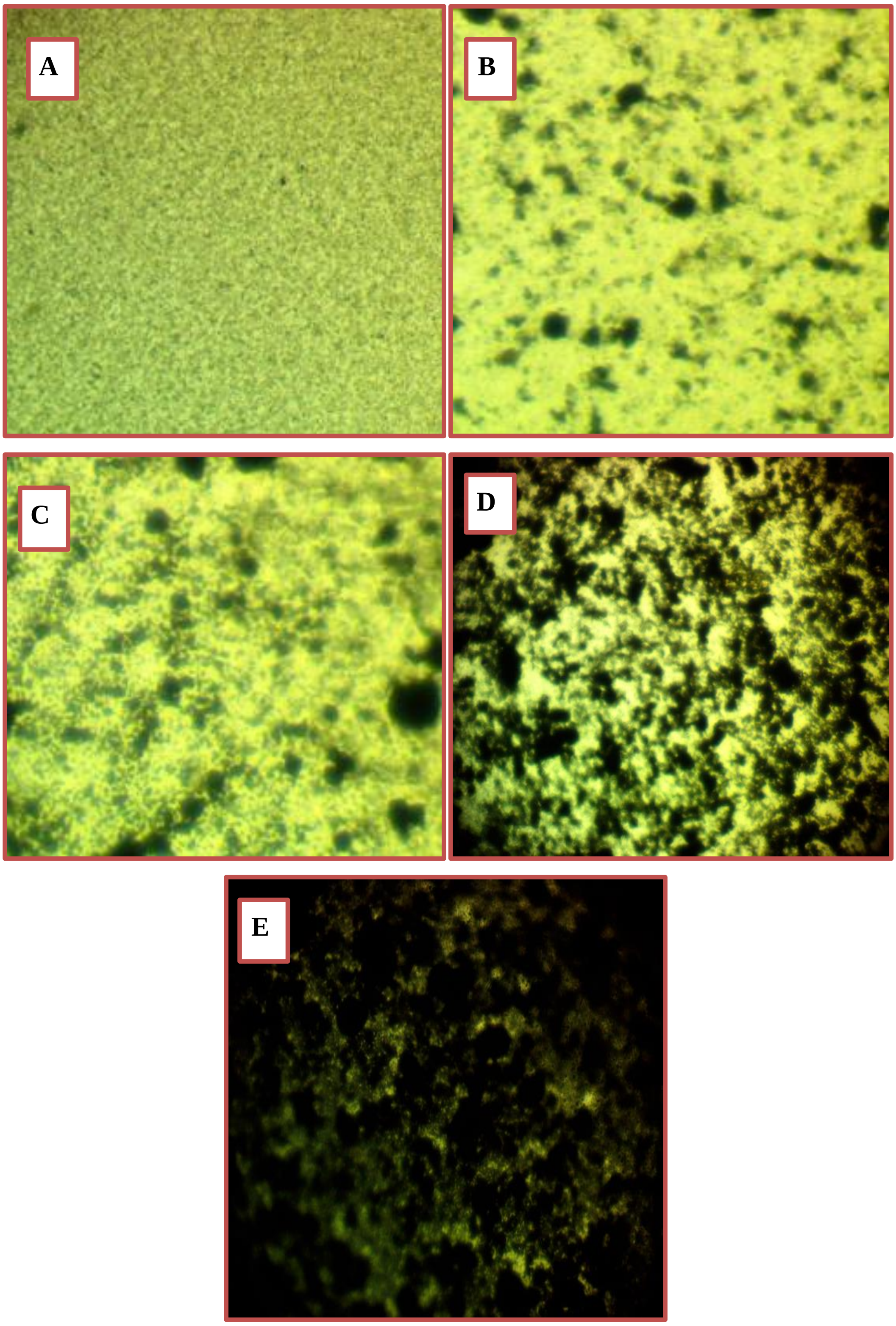
4.1 Introduction

This chapter includes the results and discussion of the structural, optical, A.C electrical properties and Applications For Antibacterial Activity of (PC/SiC-TaC) nanocomposites.

4 .2 Structural Properties of (PC/SiC-TaC) nanocomposites

4.2.1 The Optical Microscope (OM)

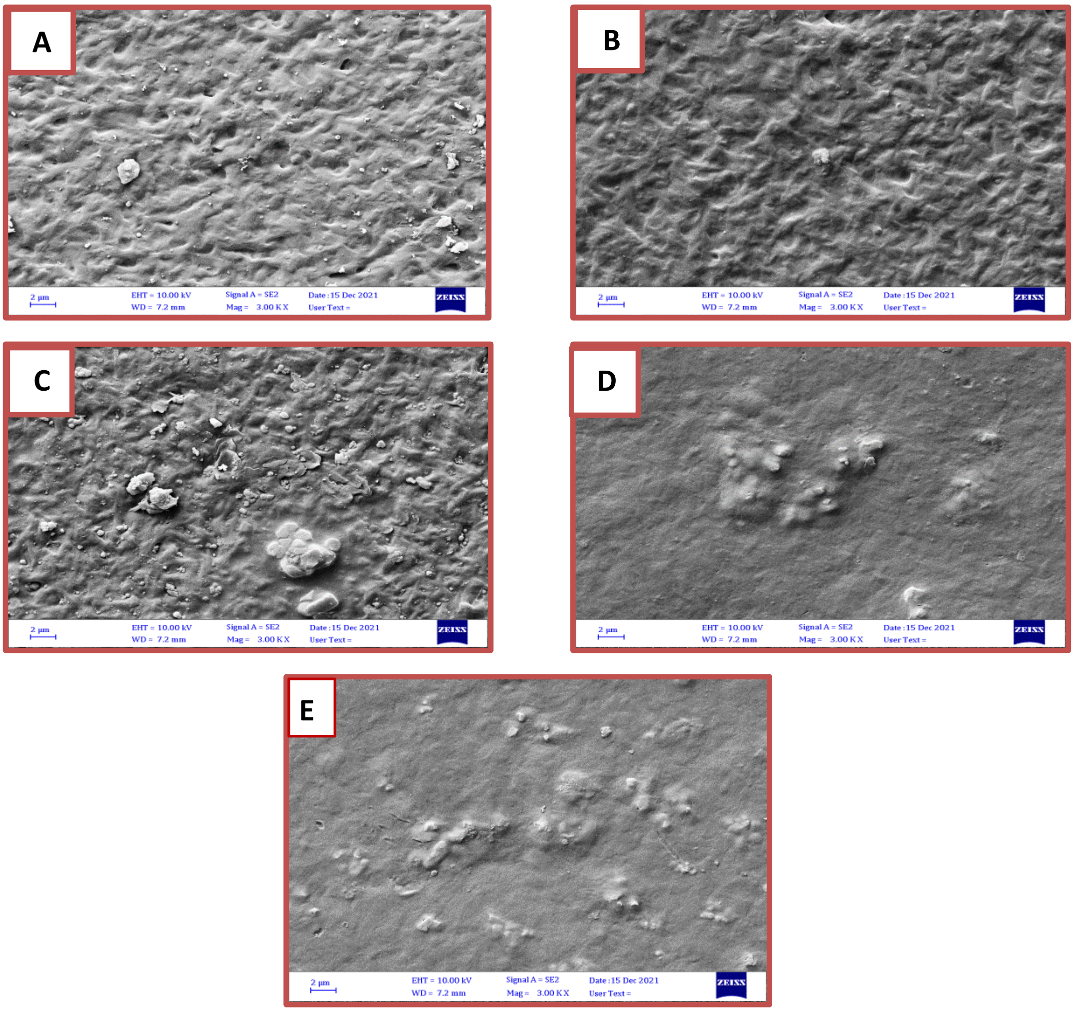
The Optical Microscope(OM) images of the pure polymer and polymer doped with (SiC-TaC) nanoparticles films at magnification (10X) with different ratio are (1.2, 2.4, 3.6, and 4.8)wt.% of (SiC,TaC) nanoparticles are shown in figure (4.1) It is indicated good homogeneity and fine incorporation of (SiC-TaC) nanoparticles in the polymer matrix. The nanoparticles form a continuous network with in the polymer matrix reached 3.6.wt% (SiC-TaC) nanoparticles, this network contains nanopaths that allow the passage of charge carriers.



Fig(4.1).Microscope images (10x): (A) PC, (B) 1.2 wt.% SiC-TaC NPs, (C) 2.4 wt.% SiC-TaC NPs, (D) 3.6 wt. % SiC-TaC NPs and (E) 4.8 wt. % SiC-TaC NPs

4.2.2 Scanning Electron Microscope (SEM) of (PC/SiC-TaC) Nanocomposites

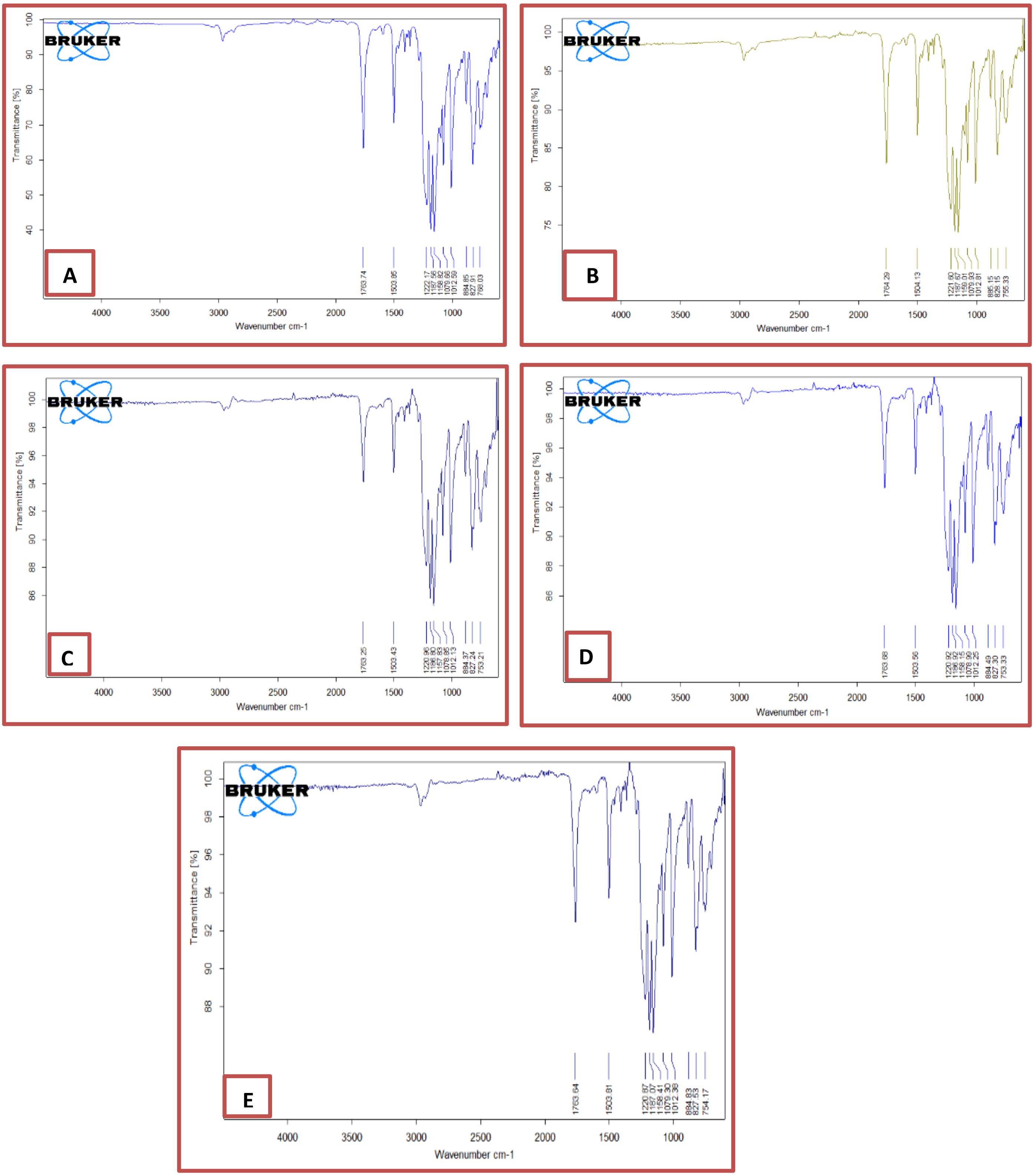
Figure (4.2) shows SEM images of (PC/SiC-TaC) at different concentrations to study the morphology of nanocomposites and arrangement of nanoparticles at higher concentrations of (SiC-TaC). SEM images show that the pathway network consists of nanoparticles within polymer matrix (PC) where charge carriers are allowed by passing through the pathways[74].This is agree with the results of the researchers[75,76].



Fig(4.2).SEM analysis of (PC/SiC-TaC) nanocomposites:(A) PC (B)1.2wt.% SiC-TaC NPs,(C)2.4 wt.% SiC-TaC NPs,(D) 3.6 wt.% SiC-TaC NPs and(E) 4.8wt.%SiC-TaC NPs

4.2.3 Fourier Transform Infrared Radiation (FTIR) of (PC/SiC-TaC) Nanocomposites

An infrared spectrometer (FTIR)is used to identify the type of bonds formed between the materials used, that is, to determine the nature of the bonds that make up the resulting mixture, in order to distinguish between a chemical reaction or a physical reaction between the materials used (PC) polymer and (SiC-TaC) nanoparticles. figure (4-3) shows the infrared spectrum of the nanocomposite (PC/SiC - TaC), as each group of infrared spectra is characteristic of certain bonds of the material within a wavenumber range ranging from (500 - 4000)cm^{-1}, The spectra curve in figure (4.3-A) is divided into three bands, where each band is represented by a group of troughs that indicate the wave numbers for each of the pure polymer bonds; As the first band, which is located in the region of bonds, is at the wave number (2700 - 3000) cm^{-1}, and the second band is at the wave number (1503 - 1763) cm^{-1} and the third band is at the wave number between (754-1222) cm^{-1}. In figure (4.3 B,C,D,E), which represents (FTIR) curves for nanocomposite films by adding (SiC - TaC) nanomaterials and by weight (1.2, 2.4, 3.6, 4.8) wt%. The infrared spectrum behavior of polymeric films after adding (SiC -TaC) is agree with its behavior in the polymeric membrane before adding (SiC-TaC) except for some slight changes resulting from the vibration of the bond, this indicates that there is no chemical reaction between the nanocomposite materials but rather aphysical reaction.



Fig(4.3).FTIR analysis of (PC/ SiC-TaC) nanocomposites:(A) PC,(B) 1.2 wt.% SiC-TaC NPs, (C)2.4 wt.% SiC-TaC NPs,(D) 3.6 wt.% SiC-TaC NPs and(E)4.8wt.%SiC-TaC NPs

4.3 The Optical Properties of (PC/SiC-TaC) Nanocomposites

The optical properties of (PC/SiC-TaC) nanocomposites include: the absorbance, transmittance, the absorption coefficient, energy band gap, extinction coefficient, reflection index, dielectric constants and optical conductivity.

4.3.1 The Absorbance and Transmittance of(PC/SiC -TaC) Nanocomposites

Figure (4.4) show the variation of absorbance for (PC/SiC-TaC) nanocomposites with wavelength of the incident light . The figure show increase of the absorption for the samples of (PC/SiC-TaC) nanocomposites at(UV region) with increasing of the concentrations for (SiC-TaC) nanoparticles , this is due to the excitations of donor level electrons to the conduction band at these energies. The high absorbance of samples for nanocomposites (PC/SiC-TaC) at UV region attributed to the energy of photon enough to interact with atoms; the electron excites from a lower to higher energy level by absorbing a photon of known energy. This behavior agree with the results of researchers[77]. At visible and near infrared regions, the absorbance of all samples for nanocomposites has low values, this behavior attributed to the energy of incident photons doesn’t enough energy to interact with atoms, thus the photons will be transmitted when the wavelength increases[78]. Figure (4.5) shows that the variation of the transmittance of (PC/SiC-TaC) nanocomposites with wavelength of the incident light . As shown in figure, the absorbance increases and the transmittance decreases with the increasing of the concentrations for (SiC-TaC) nanoparticles, this is due to the agglomeration of nanoparticles with increasing concentration and increase of the number of charge carriers[79]. The decrease in transmittance is also due to the nature of refractions and reflections within the material itself [80]. This behavior agree with the results of researchers[81,82].

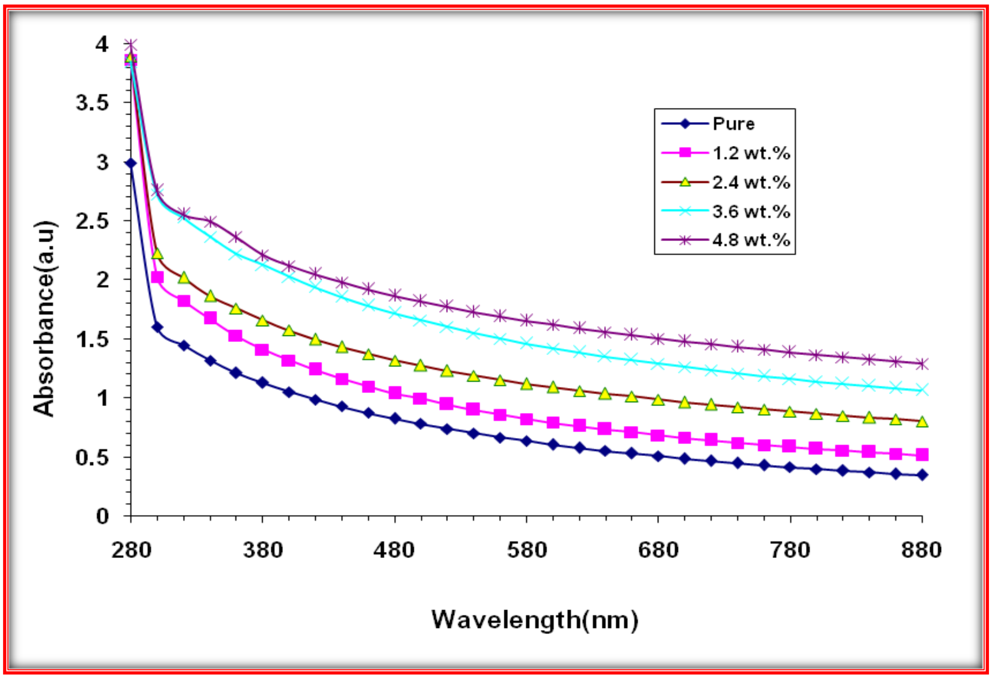


Fig.(4.4). Optical absorbance performance of PC/SiC-TaC nanostructures films with photon wavelength.

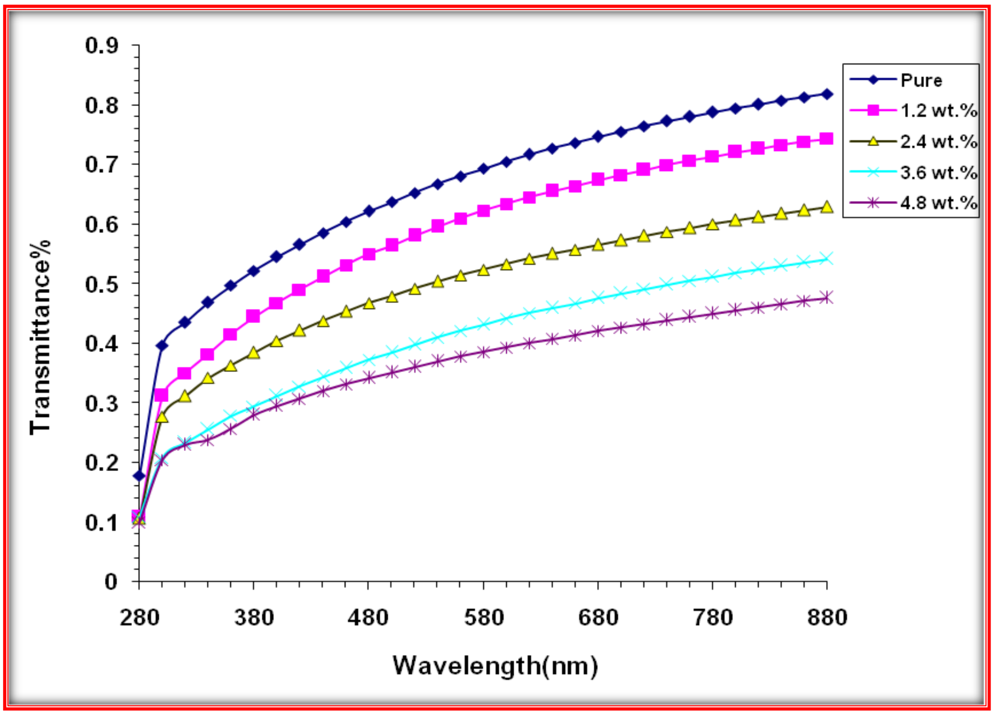


Fig.(4.5). Behavior of optical transmittance for PC/SiC-TaC nanostructures films with photon wavelength

4.3.2 The Absorption Coefficient of (PC/SiC-TaC) Nanocomposites

The absorption coefficient of nanocomposites is calculated by using equation (2-2). Figure (4.6) show the variation of absorption coefficient for (PC/SiC-TaC) nanocomposites as a function of photon energy of the incident light . As shown in the figure, the absorption coefficient of the samples for (PC/SiC-TaC) nanocomposites is high at high energies. This means that the electron transition has high possibility; i.e. the energy of incident photon is enough to transit the electron from the valence band to the conduction band which due to the energy of the incident photon is greater than the energy band gap. The absorption coefficient assists to know the nature of electron transition[83,84]. When the values of the absorption coefficient of material are high ($\alpha > 10^4$ cm^{-1}), it is expected that direct transition of electron. While, when the values of the absorption coefficient of material are low ($\alpha < 10^4$ cm^{-1}), it is expected that indirect transition of electron. The values of absorption coefficient of (PC/SiC-TaC) nanocomposites are low ($\alpha < 10^4$ cm^{-1}); the transition of electron is indirect. The absorption coefficient of nanocomposites increases with the increasing of the concentrations of nanoparticles[83].

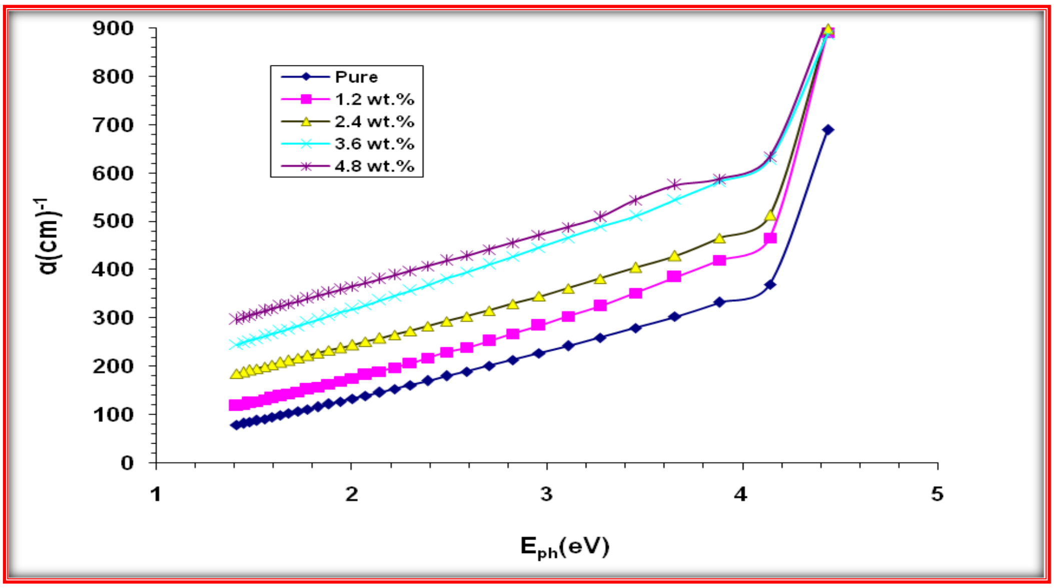
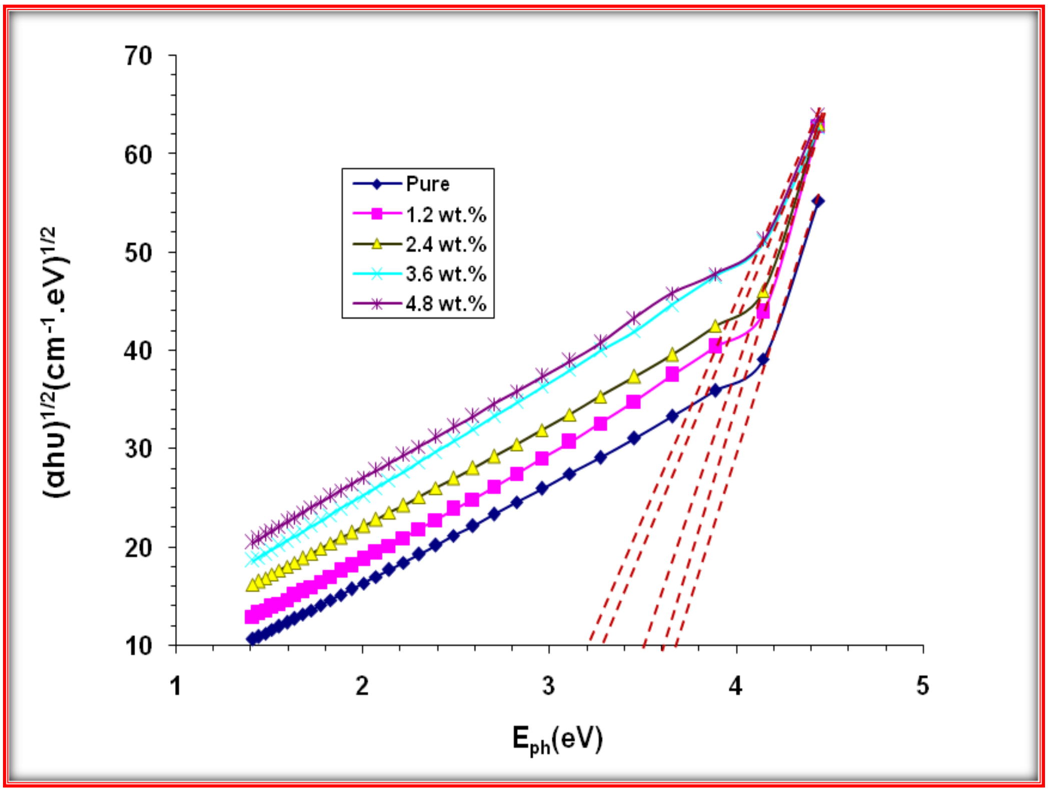


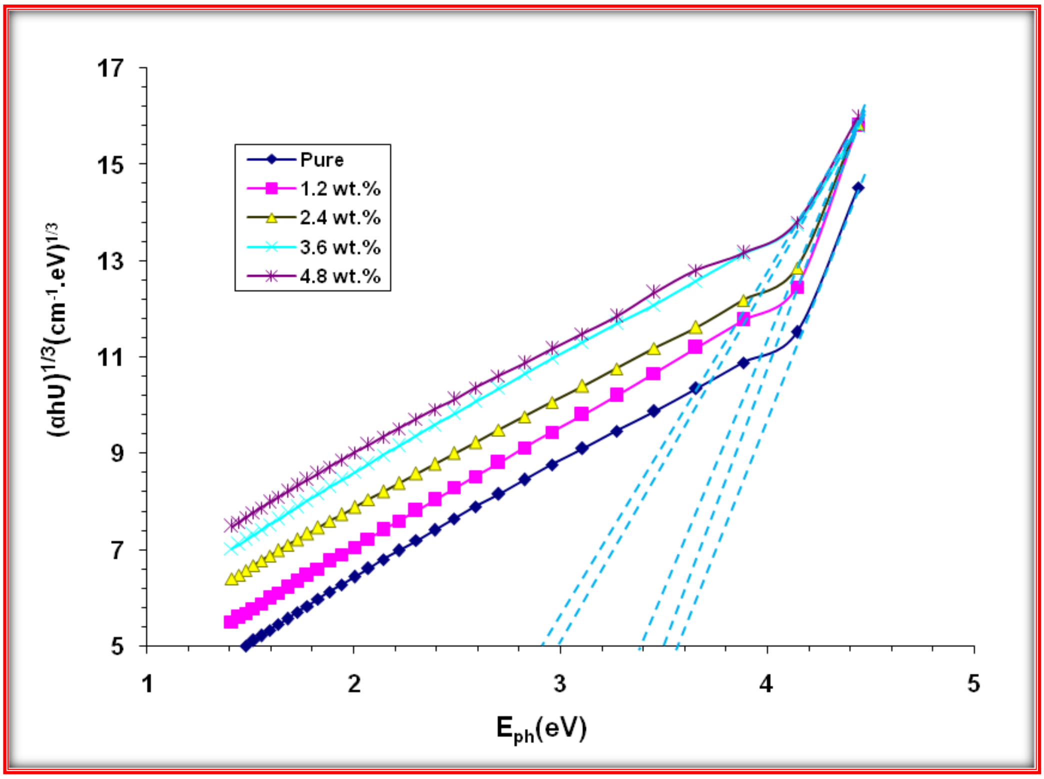
Fig.(4.6).Absorption coefficient behavior of PC/SiC-TaC nanostructures with photon energy.

4.3.3 Optical energy gap

The energy band gap of (PC/SiC-TaC)nanocomposites is calculated by using equation (2-3). The energies gaps for allowed indirect transitions of (PC/SiC-TaC) nanocomposites are shown in figure (4.7) .The energies gaps for forbidden indirect transitions of (PC/SiC-TaC) nanocomposites are shown in figure (4.8). The energies gaps for allowed and forbidden indirect transitions of (PC/SiC-TaC) nanocomposites are decreased with increasing of the (SiC-TaC) nanoparticles concentrations, this behavior is due to the creation of levels in the energy gap; the transition of electron in this case is conducted in two stages that involve the transition from the valence band to the generated levels in the energy gap and to the conduction band[85,86]. As a result of increasing the (SiC-TaC) nanoparticles concentrations. The electronic conduction depends on (SiC-TaC)nanoparticles concentrations. These results are in agreement with the results of the researcher [85,86]. The increase in the concentrations of (SiC-TaC) nanoparticles gives electronic paths in the polymer, so the electron moves from the valence band to the conduction band, which explains the decrease in the energy gap with the increase in the concentration of (SiC-TaC) nanoparticles [87]. These results agreement with previous studies[88,89]. The values of the energies gaps for allowed and forbidden indirect transformations are shown in the (4.1)table.



Fig(4.7).Energy gap values of allowed indirect transition of PC/SiC-TaC nanostructures



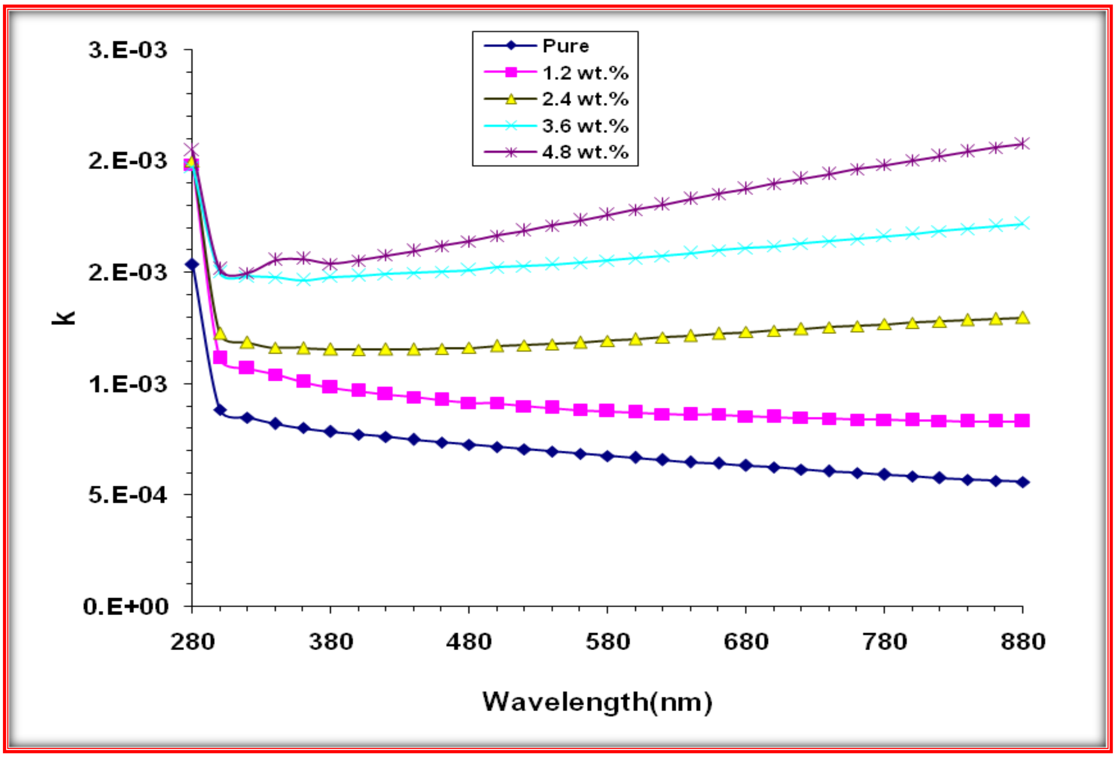
Fig(4.8). Energy gap values of forbidden indirect transition of PC/SiC-TaC nanostructures.

Table (4.1).The values of the energies gaps for allowed and forbidden indirect transformations of(PC/SiC-TaC) nanocomposites

Concentration percentage	allowable energy gap(ev)	forbidden energy gap(ev)
Pure	3.7	3.58
1.2	3.6	3.5
2.4	3.5	3.4
3.6	3.3	3
4.8	3.2	2.9

4.3.4 Extinction coefficient(K)

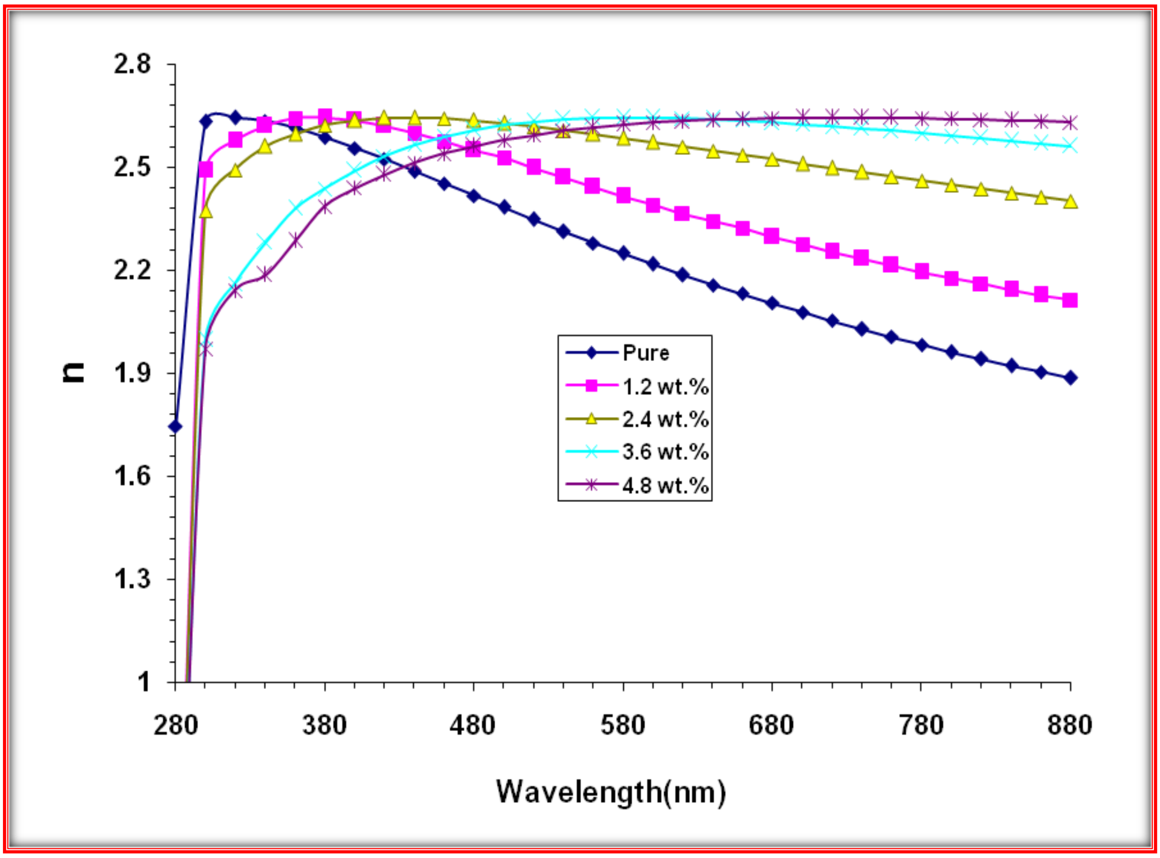
The extinction coefficient (k) of (PC/SiC - TaC) nanocomposite is calculated using equation(2-7). Figure(4-9)shows the change of the extinction coefficient as a function of wavelength. The figure show that extinction coefficient increases with increasing the concentration of (SiC-TaC) nanoparticles, this is due to the increase in optical absorption and photons dispersion in the polymer matrix[89]. Through equation (2-7) that the extinction coefficient depend on the absorption coefficient, and that the extinction coefficient has low values in the UV- region and it increases with increasing wavelength in the visible spectrum region and continues to the near infrared spectrum region. This is due to an increase in the absorption coefficient with increasing of (SiC-TaC)nanoparticles concentration. These results are in agreement with the results of the researcher [90,91].



Fig(4.9). Extinction coefficient variation of PC/SiC-TaC nanostructures with photon wavelength.

4.3.5 Refractive Index (n)

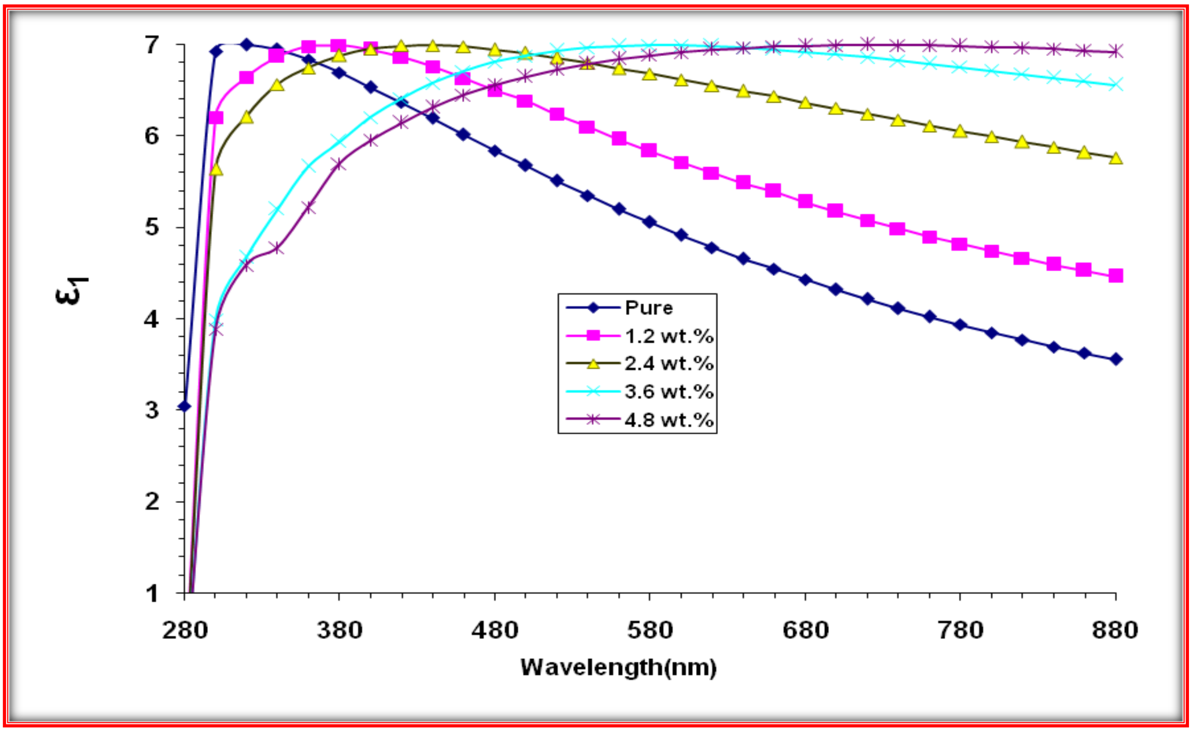
The refractive index of (PC/SiC - TaC) nanocomposite is calculated by using equation (2-8). Figure(4-10)shows the change of the refractive index as a function of wavelength. As shown in figure the refractive index of (PC/SiC-TaC) nanocomposites increases with increasing concentrations of (SiC-TaC) nanoparticles, also it is decreased with the increases of the wavelength, due to the increase in the density of nanocomposites[91]. When the incident light interacts with a sample has high refractivity at UV region, the values of refractive index will be increased. These results are in agreement with the results of the researcher[90].



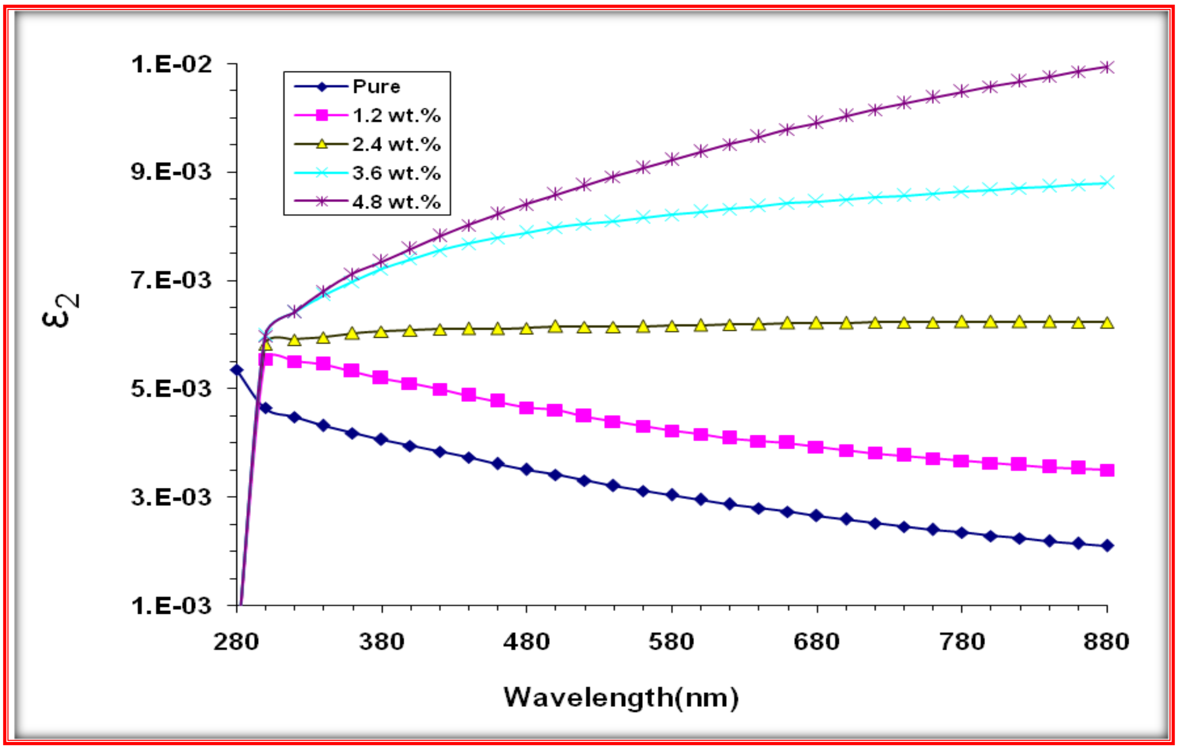
Fig(4.10). Refractive index variation of PC/SiC-TaC nanostructures with photon wavelength

4.3.6 The Real and Imaginary Parts of Dielectric Constant of Nanocomposites

The real and imaginary parts of the dielectric constant are calculated using equations (2-9) and (2-11) respectively . Figures (4.11)and (4.12) show change of the real and imaginary parts of dielectric constant with the wavelength of the (PC/SiC-TaC) nanocomposites. The figure (4.11) shows change of the real parts of the dielectric constant of (PC/SiC-TaC) with wavelength. The real part of the dielectric constant depends on the refractive index because the extinction coefficient is very small. so, real dielectric constant is increased with increase of the (SiC-TaC) nanoparticles concentrations[78]. The effect of (SiC-TaC) nanoparticles on the imaginary part of dielectric constant is shown in Figure(4.12) .The figure shows that imaginary part of dielectric constant of (PC/SiC-TaC) nanocomposites are increased with increasing of (SiC-TaC) nanoparticles concentrations, this behavior attributed to the increase of electrical polarization, due to contribution of nanoparticles concentration in the sample and increase in charges within the polymers[92].The imaginary part of dielectric constant depends on extinction coefficient especially in the visible and near infrared regions of wavelength, where the refractive index is approximately constant while extinction coefficient increases with the increase of the wavelength[93].



Fig(4.11).Behavior of real part of dielectric constant for PC/SiC-TaC nanostructures with photon wavelength



Fig(4.12).Behavior of imaginary part of dielectric constant for PC/SiC-TaC nanostructures with photon wavelength

4.3.7 Optical Conductivity

Figure (4.13) shows the variation of optical conductivity with wavelength for (PC/SiC-TaC) nanocomposites .The optical conductivity of nanocomposites are decreased with the increasing of the wavelength, this behavior attributed to the optical conductivity depends on the wavelength of the radiation incident on the samples of nanocomposites.The increase of optical conductivity at low wavelength of photon is due to high absorbance of nanocomposites in that region. Also, the optical conductivity of nanocomposites is increased with the increase of nanoparticles concentrations, this behavior related to the creation of localized levels in the energy gap;hence, increase of the absorption coefficient and increasing the optical conductivity of nanocomposites[94].

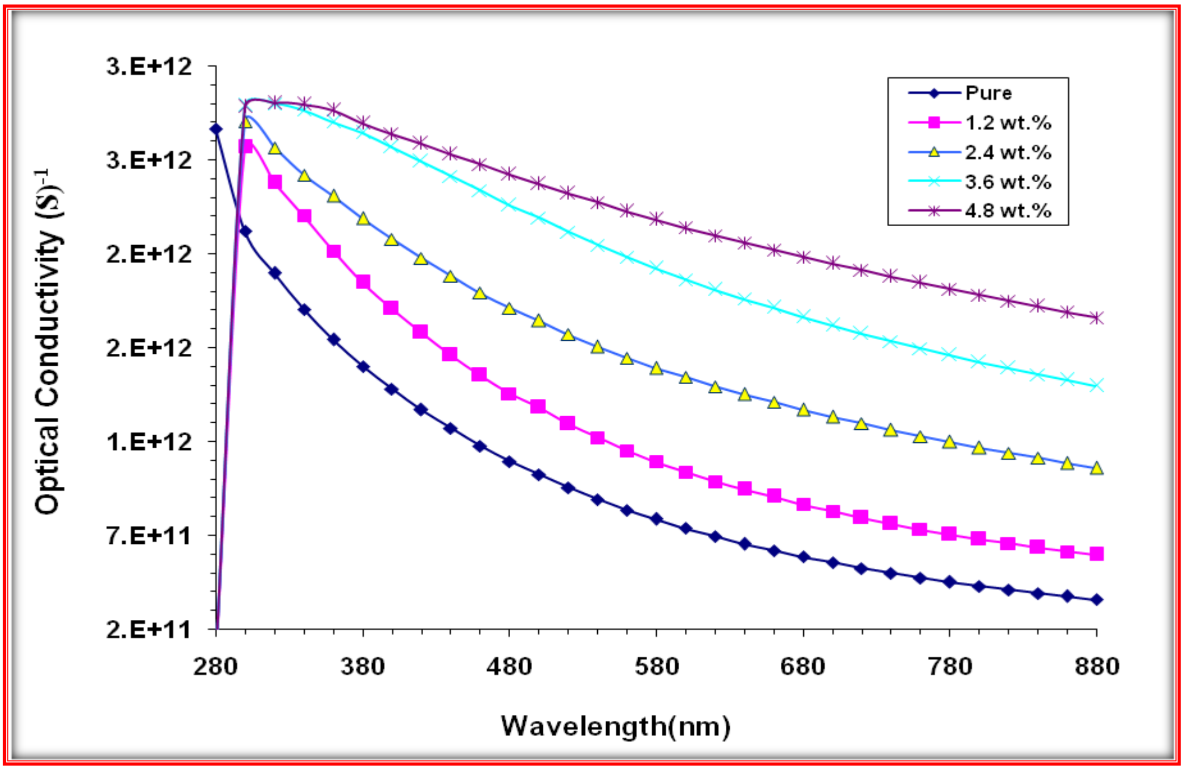


Fig.(4.13).Optical conductivity performance of PC/SiC-TaC nanostructures with wavelength.

4.4 The A.C Electrical Properties of (PC/SiC-TaC) Nanocomposites

The A.C electrical properties of the nanocomposite (PC/SiC-TaC) were studied in the range of frequencies between (100 - 5×10^{6})Hz and the dielectric constant was calculated using the equation (2-19) , and the dielectric loss using the equation (2-20) and the A.C electrical conductivity is calculated for nanocomposites by using equation (2.21).

4.4.1 The Dielectric Constant of (PC/SiC-TaC) Nanocomposites

Figure (4.14) shows the effect of adding the (SiC-TaC) nanoparticles concentration on the values of the dielectric constant at (100Hz) and room temperature. The increase in the concentration of (SiC-TaC) nanoparticles leads to an increase the dielectric constant. This behavior could be interpreted from interfacial polarization inside the nanocomposites in applied alternating electric field and the increasing of the charge carriers[95]. At low concentrations of (SiC-TaC) nanoparticles are in separate groups from each other, there will be a small increase in the dielectric constant. Increase concentration of (SiC-TaC) nanoparticles, these materials will generate a connected network inside the polymeric material, causing an increase in the charge carriers for increase the polarized charges, and as a result, the dielectric constant increases [95,96]. Figure (4.15) shows the effect of the frequency of the electric field on the dielectric constant of the nanocomposite (PC/SiC-TaC), that the dielectric constant decreases when the frequency of the applied field increases, and the reason for this is that the dipoles of the nanocomposites go in the direction of the applied electric field, so the polarization of the space charge decreases to the total polarization[97]. the space charge polarization becomes the more contributing of polarization at low frequencies, and less contributing with the increase of frequency, this causing decrease in dielectric constant values for all samples of (PC/SiC-TaC) nanocomposites with the increase of the electric field frequency. [98]. The ionic polarization reacts slightly to the variation in the field frequencies compared with electronic polarization, this is because the mass of ion is greater than that of the electron. The electrons respond to even the high frequencies of the field vibrations. This is agree with the results of the researchers [98].

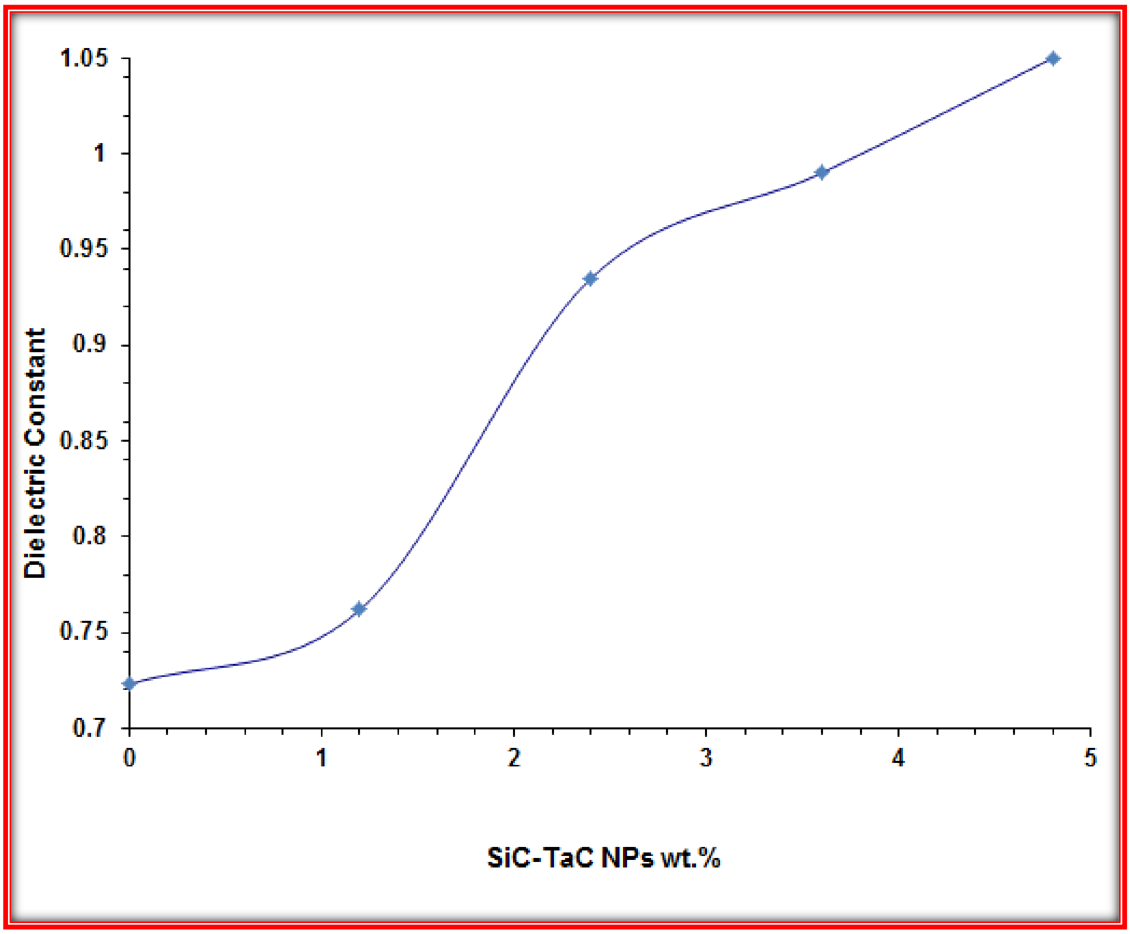


Fig. (4.14). Effect of (SiC-TaC) nanoparticles concentrations on dielectric constant for (PC/SiC-TaC) nanocomposites at (100Hz)

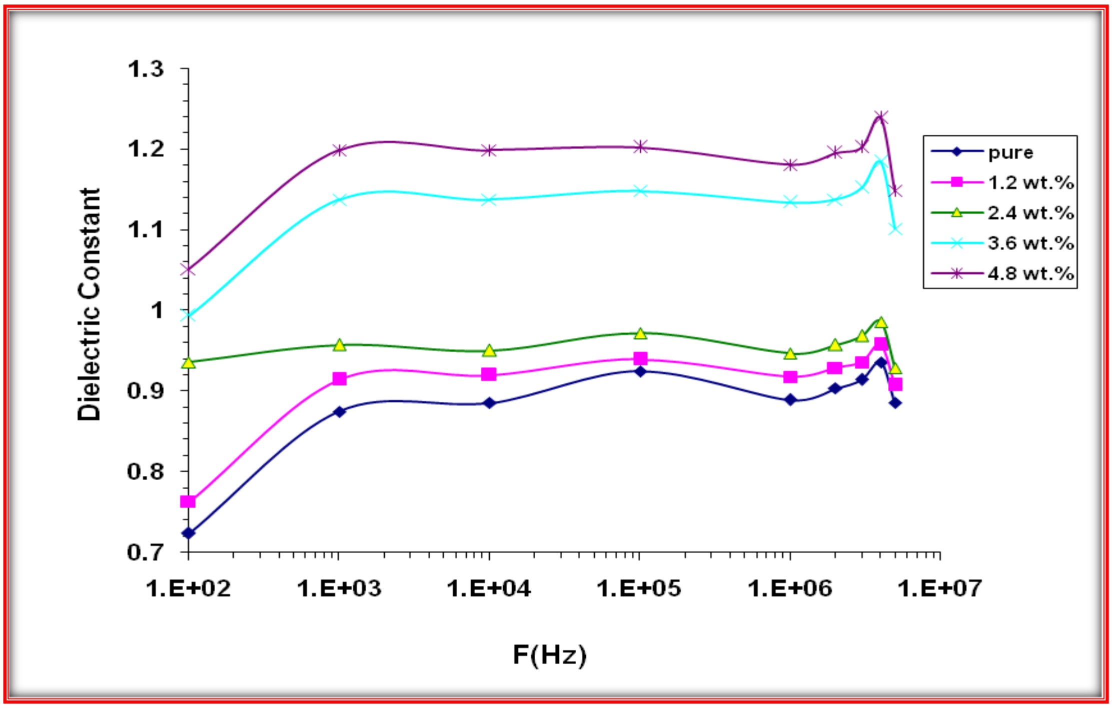


Fig.(4.15). Behavior of dielectric constant of PC/SiC-TaC nanostructures against frequency

4.4.2 The Dielectric Loss of (PC/SiC-TaC) Nanocomposites

Figure (4.16) shows the change of dielectric loss with increasing of the (SiC-TaC) nanoparticles concentrations. The dielectric loss increases with increasing of the (SiC-TaC) nanoparticles ratios concentrations, due to the increase of charge carriers. At low concentrations of nanoparticles, it forms clusters shape. When the concentration of nanoparticles reaches to (3.6 and 4.8) wt.%, the nanoparticles form a continuous network in the nanocomposites. This is agree with the results of the researchers [98,99]. Figure (4.17) shows the variation of the dielectric loss of (PC/SiC-TaC) nanocomposites with frequency of applied electric field. When the frequency of the applied field is small, the dielectric loss will increase, and its value will decrease with the increase in frequency due to the decrease in the interpolarization (decrease of the space charge polarization) with increasing frequency . The figure also shows that the highest amount of dielectric loss at the frequency (100 Hz) compared to the occurrence of the highest absorption of the applied electric field according to "Maxwell-Weekner principle". At a certain value of the frequency (4×10^6 Hz) the electric current and the applied field become the same phase, so the dielectric loss becomes constant due to a type of polarization at those frequencies high This is agree with the results of the researchers[98].

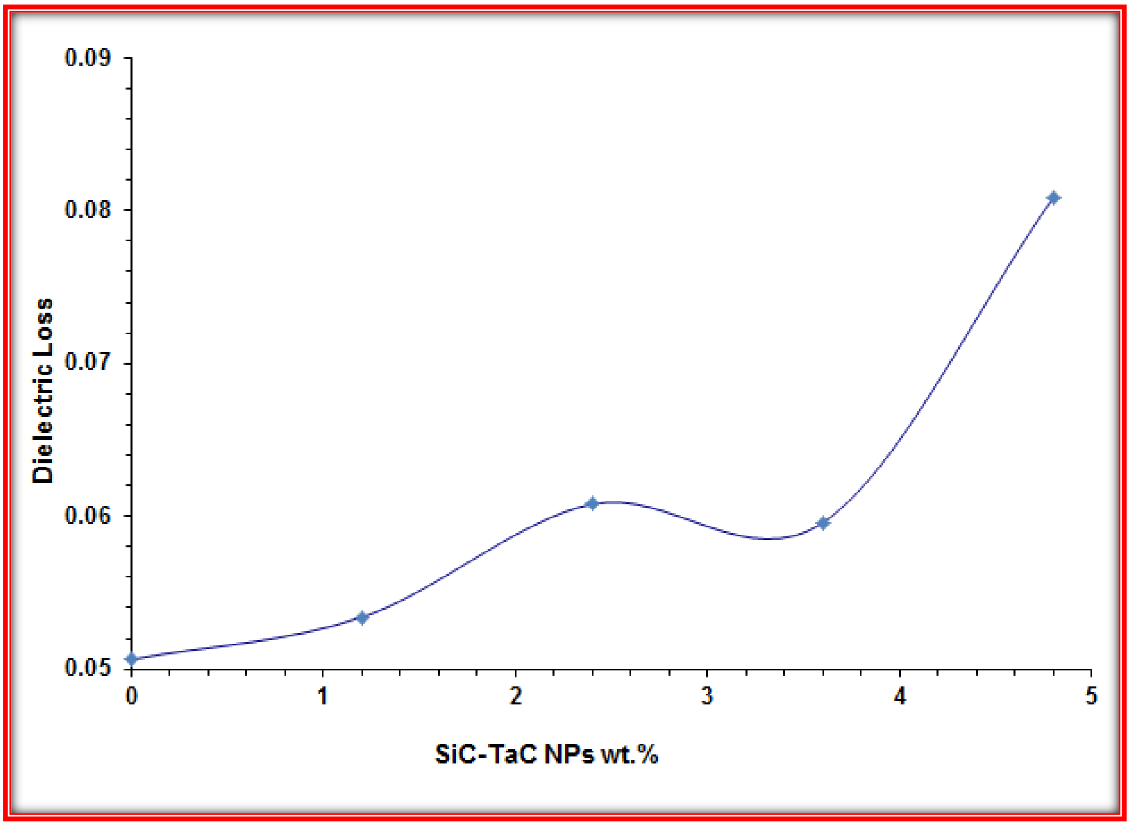


Fig. (4.16). Effect of (SiC-TaC) nanoparticles concentrations on dielectric loss for (PC/SiC-TaC) nanocomposites at (100Hz)

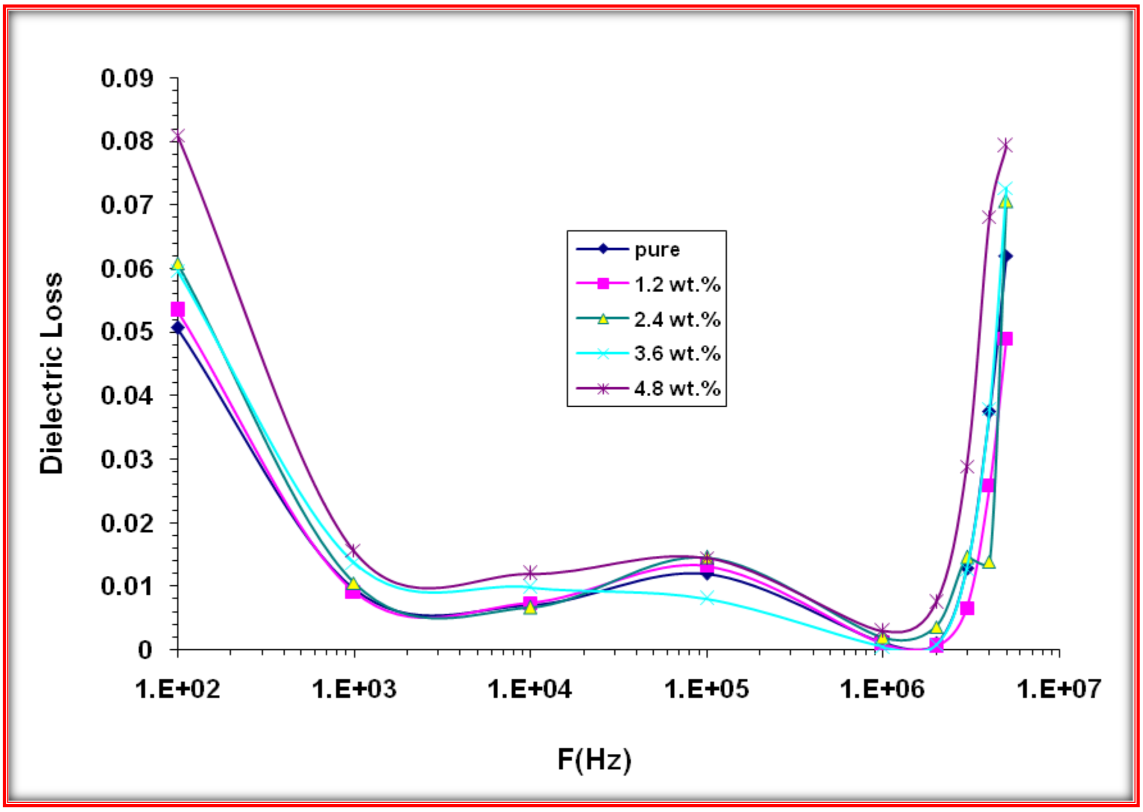


Fig.(4.17). Dielectric loss of PC/SiC-TaC nanosystem against frequency.

4.4.3 The A.C Electrical Conductivity (PC/SiC-TaC) Nanocomposites

The A.C electrical conductivity ($\sigma_{A.C}$) of the (PC/SiC-TaC) nanocomposite is calculated from the relationship (2-21). Figure (4.18) shows the change of the A.C electrical conductivity ($\sigma_{A.C}$) of the(PC/SiC-TaC)nanocomposite with the change in the concentrations of (SiC-TaC) nanoparticles at the frequency (100 Hz). The A.C electrical conductivity of (PC/SiC-TaC) increases with the increase in (SiC-TaC) nanoparticle concentrations. The increase in the A.C electrical conductivity results from the increase in the number of charge carriers, so the resistance of the (PC/SiC-TaC) nanocomposite decreases due to the nanoparticles structure. When the concentration of nanoparticles reaches to (3.6 and 4.8) wt.%, the nanoparticles form a continuous network in the nanocomposites[99,100]. Figure (4.19) shows the change of The A.C electrical conductivity of the (PC/SiC-TaC) nanocomposite with the change of frequency at room temperature. The A.C electrical conductivity increases with the increase in the frequency of the applied electric field for all nanocomposite samples. This behavior is attributed to the mobility of charge carriers and the hopping of ions from the cluster. The charge carriers move higher in the higher frequency region, hence the electrical conductivity increases with frequency for the nanocomposites[101].This behavior is agree with the results of the researcher[102].

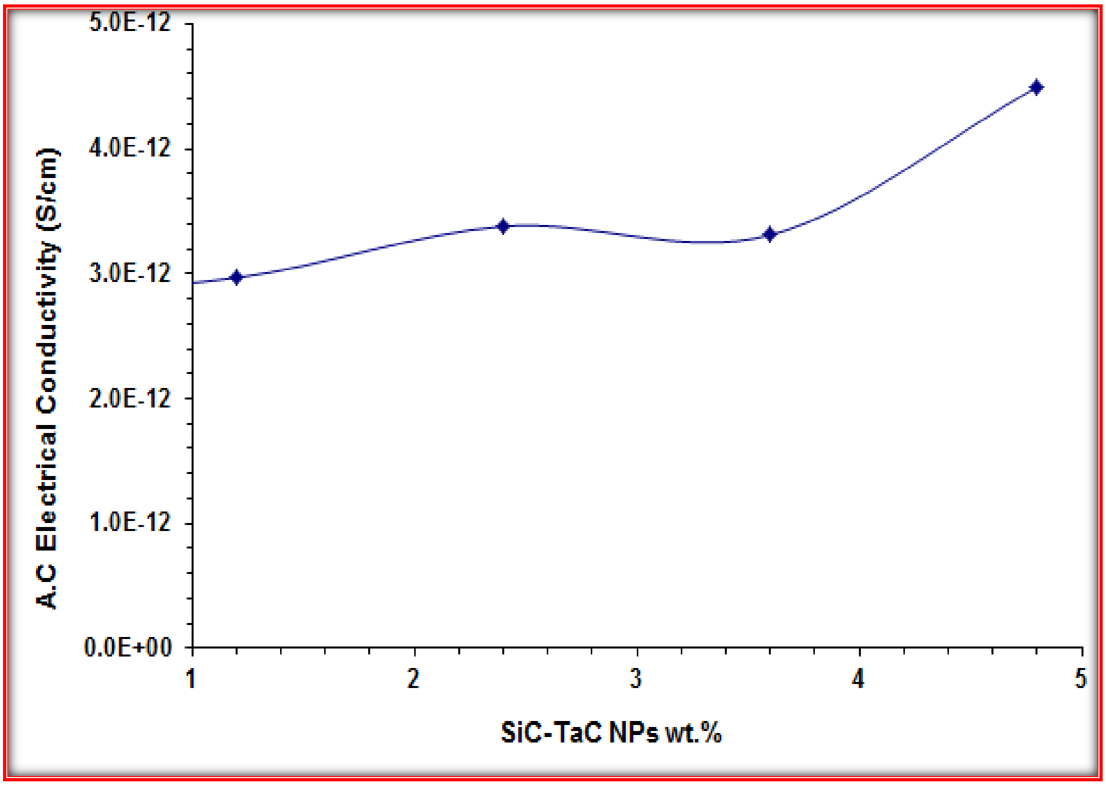


Fig. (4.18). Effect of(SiC-TaC) nanoparticles concentrations on A.C electrical conductivity for (PC/SiC-TaC) nanocomposites at 100Hz

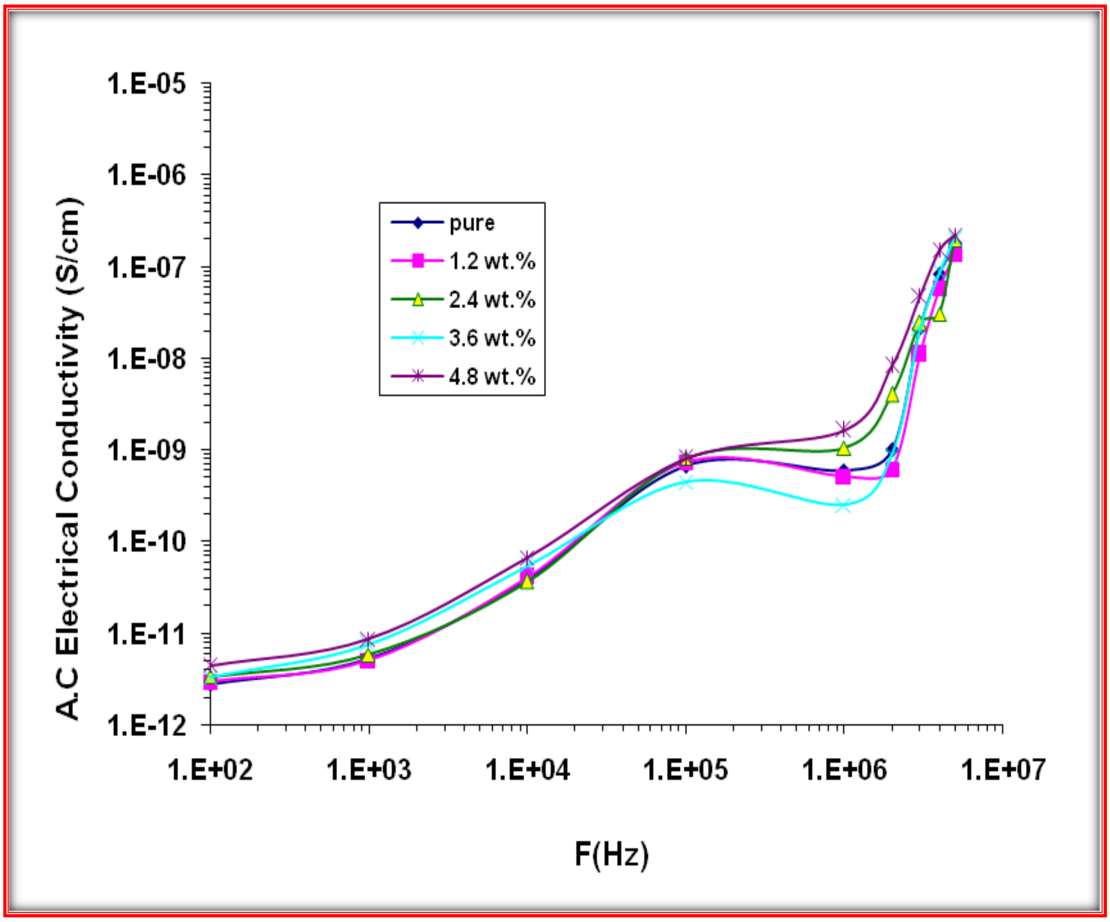


Fig. (4.19). Variation of A.C electrical conductivity for (PC/SiC-TaC) nanocomposites with frequency at room temperature.

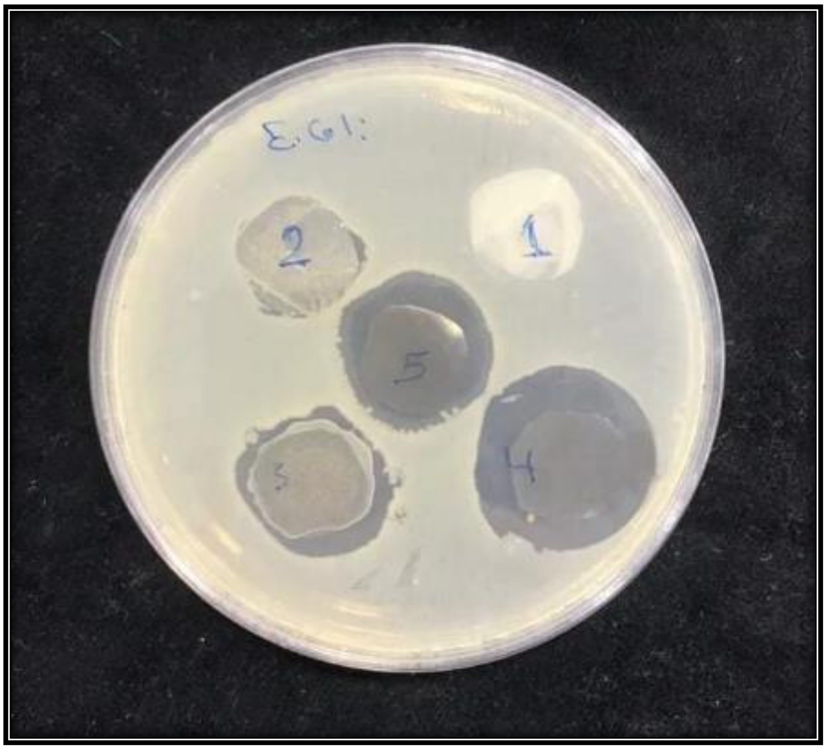
4.5 Applications of (PC/SiC-TaC) Nanocomposites For Antibacterial Activity

The antibacterial properties of the (PC/SiC-TaC) nanocomposites were tested against gram-positive (Staphylococcus aureus) and gram-negative (Escherichia coli) and the obtained data are presented in Figure (4.20) and figure (4.21). As shown in the figures, the inhibition zone increases with increasing the concentrations of (SiC-TaC) nanoparticles.The reason for the bactericidal activity of nanostructures is due to the presence of (ROS)reactive oxygen species generated by nanoparticles [103]. The nanocomposites are carrying the positive charges and the microbes are having the negative charges, which create the electromagnetic attraction between the nanoparticles of nanocomposites and the microbes,will the microbes get oxidized and die instantly [104]. The main mechanism that caused the antibacterial activity of nanocomposites by the nanoparticles , ROS includes radicals like super oxide radicals (O^{-2}), hydroxyl radicals (OH) and hydrogen peroxide (H_2O_2); and singlet oxygen ($^1O_2$) could be the reason damaging the proteins and DNA of bacteria[103,105]. The table shows the inhibition zone diameter of (PC/SiC-TaC) nanocomposites.

Table (4.2). inhibition zone diameter of (PC/SiC-TaC) nanocomposites

Number of samples	Staphylococcus aureus(mm)	Escherichia coli(mm)
1	0	0
2	16	18
3	19	22
4	20	23
5	21	27

Fig(4.20). inhibition zone diameter image of Staphylococcus aureus (1)PC (2)1.2wt.% SiC-TaC NPs(3)2.4 wt.% SiC-TaC NPs(4)3.6 wt. % SiC-TaC NPs (5) 4.8 wt. % SiC-TaC



Fig(4.21). inhibition zone diameter image of Escherichia coli (1)PC (2)1.2wt.% SiC-TaC NPs(3)2.4 wt.% SiC-TaC NPs(4)3.6 wt. % SiC-TaC NPs (5) 4.8 wt. % SiC-TaC NPs

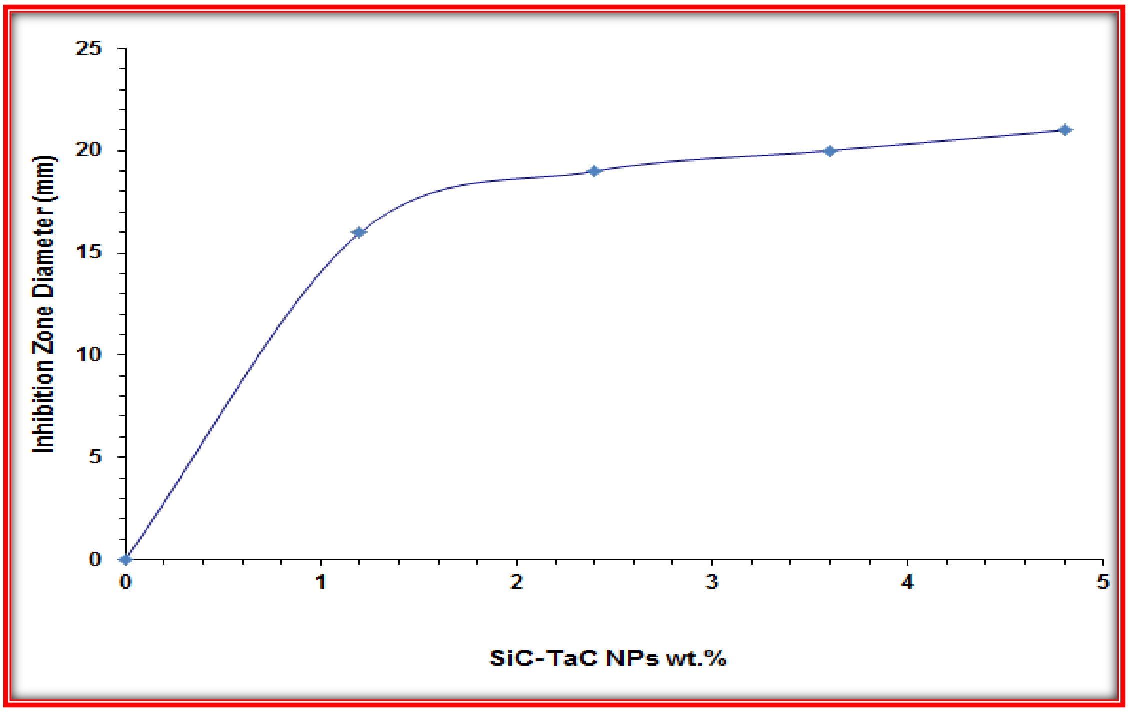


Fig. (4.22). Antibacterial effect of (PC/SiC-TaC) as a function of (SiC-TaC) nanoparticles concentrations on S. aureus.

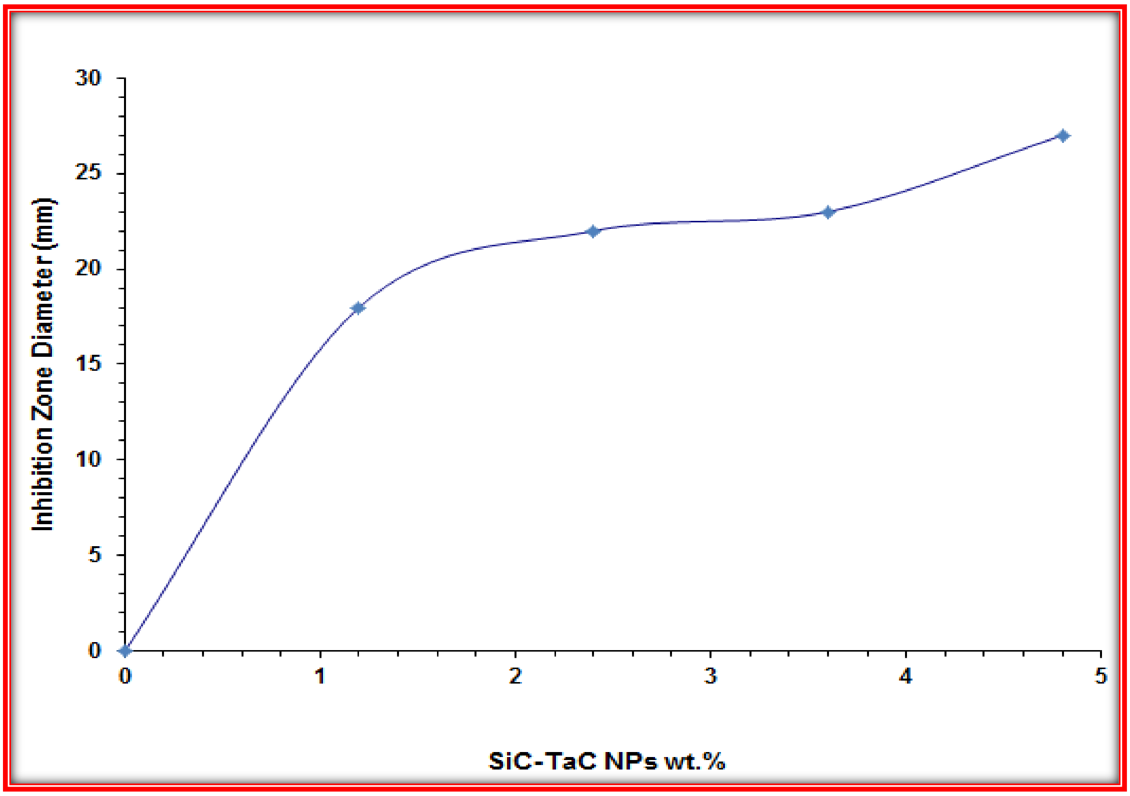


Fig. (4.23). Antibacterial effect of (PC/SiC-TaC) as a function of (SiC-TaC) nanoparticles concentrations on E. coli.

4.6 Conclusions

1.The optical microscope images showed the (SiC-TaC) nanoparticles form continuous network inside at concentration (3.6 and 4.8)wt.%. The FTIR measurements indicate vibration bands for polymer before and after addition (SiC-TaC) nanoparticles, and that the polymer after addition may have formed chains networks of polymer nanocomposites and their effects appeared in electrical and optical properties.

2.The absorbance increases with increasing concentration of (SiC-TaC) the additive, while the Transmittance decreases with increasing concentration of the additive. The absorbance is high in the UV region and the absorbance is very low in the visible region. The optical properties of (PC/SiC-TaC)nanocomposite. contain refractive index (n), extinction coefficient (K), and the dielectric constant (real and imaginary) part, increase with increasing the concentration of (SiC-TaC), the best results were at concentration (4.8)wt.% of nanoparticles. The absorption coefficient (PC/SiC-TaC) nanocomposites is less than (10^4 cm^{-1}) at all concentrations and from these, the result is being indirect transition. The energy gap for indirect transition (allowed, forbidden) decreases with increases the concentration of (SiC-TaC) nanoparticles. It can be used in the manufacture of smart windows, optical and electrics devices.

3.The dielectric constant and the dielectric loss of the (PC/SiC-TaC) nanocomposites decrease with the increase in frequency of the applied electric field, while the A.C electrical conductivity increases with increase of the frequency. The dielectric constant , dielectric loss and A.C electrical conductivity of (PC/SiC-TaC) nanocomposites increases with increasing of (SiC-TaC) nanoparticles concentrations, the best results were at concentration(4.8)wt.% of nanoparticles. It can be used in the manufacture of the sensors, and electrical energy storage devices such as capacitors.

4.The results of antibacterial application for (PC/SiC-TaC) nanocomposites showed that the inhibition zone for S. aureus and E. coli an increases with an increase concentrations of (SiC-TaC) nanoparticles which may be used it for antibacterial with high activity.

4.7 Future works

1.Studying the effect of (SiC-TaC) nanoparticles on thermal conductivity.

2.Study of mechanical properties of (PC/SiC-TaC) nanocomposites

3.Studying the effect of temperature on dielectric properties of (PC/SiC-TaC) nanocomposites.

4.Study of pressure sensors application of (PC/SiC-TaC) nanocomposites

5.Study of humidity sensors application of (PC/SiC-TaC) nanocomposites .

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الخلاصة

تم تحضير المركبات النانوية (PC/SiC-TaC) بطريقة الصب المحلول. تمت دراسة تأثير تراكيز الجسيمات النانوية (SiC-TaC) على الخواص التركيبية والبصرية والكهربائية للمركبات النانوية (PC/SiC-TaC) وتطبيقاتها كنشاط مضاد للجراثيم. أظهرت النتائج التجريبية للخصائص التركيبية للمركبات النانوية (PC/SiC-TaC) التجانس الجيد والدمج الدقيق للجسيمات النانوية (SiC-TaC) في مصفوفة البوليمر ، وتشكل الجسيمات النانوية شبكة مستمرة داخل مصفوفة البوليمر ، وتحتوي هذه الشبكة على مسارات تسمح بمرور ناقلات الشحنة. يتوافق سلوك طيف الأشعة تحت الحمراء للأغشية البوليمرية بعد إضافة (SiC-TaC) مع سلوكها في الغشاء البوليمري قبل إضافة (SiC-TaC) باستثناء بعض التغييرات الطفيفة الناتجة عن اهتزاز الاصرة ، وهذا يشير إلى عدم وجود تفاعل كيميائي بين المواد المخلوطة بل تفاعل فيزيائي. أظهرت النتائج التجريبية للخواص البصرية للمركبات النانوية (PC/SiC-TaC) زيادة معامل الامتصاص ومعامل الخمود ومعامل الانكسار وثوابت العزل الحقيقية والخيالية والتوصيلية البصرية للمركبات النانوية (PC/SiC-TaC) بزيادة تراكيز الجسيمات النانوية (SiC-TaC). تم تقليل فجوة نطاق الطاقة والنفاذية مع زيادة تراكيز الجسيمات النانوية (SiC-TaC). تتميز المركبات النانوية (PC/SiC-TaC) بامتصاص عالي في منطقة الأشعة فوق البنفسجية. تمت دراسة الخواص الكهربائية للتيار المتردد للمركبات النانوية (PC/SiC-TaC) بتردد يتراوح ($10^6 \times 5 - 100$) هرتز عند درجة حرارة الغرفة. أظهرت النتائج التجريبية أن ثابت العزل وفقد العزل الكهربائي للمركبات النانوية (PC/SiC-TaC) انخفض مع زيادة تردد المجال الكهربائي المطبق. تزداد الموصلية الكهربائية للتيار المتردد مع زيادة التردد. تمت زيادة ثابت العزل وفقد العازل والتوصيل الكهربائي للمركبات النانوية (PC/SiC-TaC) مع زيادة تراكيز الجسيمات النانوية (SiC-TaC). أظهرت نتائج التطبيقات المضادة للبكتيريا للمركبات النانوية (PC/SiC-TaC) التي تم اختبارها ضد موجبة الجرام (S. aureus) وسالبة الجرام (E. coli) زيادة منطقة التثبيط مع زيادة تراكيز الجسيمات النانوية (SiC-TaC).

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تحسين الخصائص التركيبية، البصرية والكهربائية لبوليمر حيوي مشوب بكاربيدات نانوية للتطبيقات المضادة للبكتيريا

رسالة مقدمة

إلى مجلس كلية التربية للعلوم الصرفة في جامعة بابل وهي جزء من متطلبات درجة الماجستير في التربية\ الفيزياء

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2022م 1443هـ