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Investigation of Structural, Optical and Electrical Characteristics of Polymeric Nanocomposites as Antibacterial Application

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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2023 A.D **1444 A.H**

بسم الله الرحمن الرحيم

{شَهِدَ اللّهُ أَنَّهُ لاَ إِلَـهَ إِلاَّ هُوَ وَالْمَلاَئِكَةُ
وَأُوْلُواْ الْعِلْمِ قَآئِمَاً بِالْقِسْطِ لاَ إِلَـهَ إِلاَّ هُوَ
الْعَزِيزُ الْحَكِيـمُ}

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قسم الفيزياء

استقصاء الخصائص التركيبية والبصرية والكهربائية للمتراكبات النانوية البوليمرية وتطبيقها كمضاد بكتيري

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الخلاصة

في هذه الدراسة تم تحضير المتراكبات النانوية ($Ps/SiC/Sb_2O_3$) بطريقة الصب بتراكيز مختلفة من كربيد السيليكون واكسيد الانتيمون الثلاثي النانوية لدراسة الخصائص التركيبية والبصرية وكذلك الكهربائية للمتراكبات النانوية لاستخدامه كمضاد للبكتريا. الخصائص التركيبية تشمل المجهر الضوئي(OM),والمجهر الالكتروني الماسح(FE-SEM),وتحويل فورييه للأشعة تحت الحمراء(FTIR),اظهرت صور المجهر الضوئي انه مع زيادة تراكيز الجسيمات النانوية تتشكل شبكة مستمره داخل المصفوفة البوليمرية التي تعمل بمثابة ناقلات للشحنة, واظهرت نتائج قياس (FE-SEM)التوزيع الجيد والمتجانس للجسيمات النانوية على مورووفولوجيا السطح, أما نتائج(FTIR)فقد اشارت الى حصول تفاعل فيزيائي بين المصفوفة البوليمرية والجسيمات النانوية, اما نتائج الخصائص البصرية للمتراكبات النانوية($PS/SiC/Sb_2O_3$)اظهرت ان الامتصاصية ومعامل الامتصاص ومعامل الخمود ومعامل الانكسار وثوابت العزل الحقيقي والخيالي وكذلك الموصلية البصرية تزداد مع زيادة تراكيز الجسيمات النانوية(SiC/Sb_2O_3)بينما فجوة الطاقة والنفاذية تقل مع زيادتها, أظهرت نتائج الخواص الكهربائية للمتراكبات النانوية أن ثابت العزل والفقد الكهربائي تقل مع زيادة التردد الكهربائي المسلط وتزداد مع زيادة التراكيز للجسيمات النانوية(SiC/Sb_2O_3)بينما تزداد الموصلية الكهربائية مع زيادة التردد وزيادة التراكيز للجسيمات النانوية.اظهرت نتائج التطبيقات للمتراكبات النانوية($PS/Sic/Sb_2O_3$)ضد البكتريا ان قطر منطقة التثبيط يزداد مع زيادة تراكيزالجسيمات النانوية.

Supervisor Certification

I certify that this thesis entitled **“Investigation of Structural, Optical and Electrical Characteristics of Polymeric Nanocomposites as Antibacterial Application"** is prepared by the student **(Nawras Karim Abd Moein Battah)** under my supervision at the College of Education for Pure Sciences, University of Babylon as partial fulfillment of the requirements for the Degree of Master in Education / Physics.

Signature:
Name: Dr. Majeed. A. Habeeb
Title: Professor
(Supervisor)
Date: /   / 2023

Head of the Department Certificate

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

Signature:

Name: Dr. Khalid .H. Abbas

Title: Professor

Head of Physics Department

Date: /   /2023

Dedication

To the memory of my beloved mother

To my heaven and my only army, to my mother, who passed away without obtaining the fruits of her giving, and Her memory remained fragrant accompanying my steps. My dear mother, I dedicate to your pure soul the reward of this manger, and pray To God that it be written in your good deeds. Without your perseverance and Effort in urging me to choose the right thing, I would not be here.

Nawrs

Acknowledgments

In the Name of Allah, the Compassionate, the Merciful.

First, thanks to Allah, the Lord of Earth and Heaven for Completing

My research, then, I would like to express my deep gratitude and Appreciation to my supervisor. Prof. Dr. Majeed Ali Habeeb for suggesting this project, guidance, support, and encouragement through the research work. I also would like to express gratitude to all teachers, instructors and students of the department of physics for their assistance and supports especially Eventually, Many thanks to those who always support me and alleviate the difficulties I have faced during my works and everyone who helped me in a way or another during my preparation of this thesis. I apologize for who I miss mentioning. I wish success to all.

Nawrs

Abstract

The nanocomposites of ($PS/SiC/Sb_2O_3$) were prepared by casting method with different concentrations of SiC and Sb_2O_3 nanoparticles to study the structure, and optical and electrical properties of nanocomposites for antibacterial application. The structural properties studied include optical Microscope (OM)field emission, Scanning electron microscope (FE-SEM), and Fourier transforms infrared (FT-IR). The optical microscopy images showed that with increasing concentrations of nanoparticles, network paths are formed inside the polymeric matrix that act as charge carriers. And FE-SEM measurement results showed a good distribution and homogeneous surface morphology. The results of FT-IR indicate a physical interference between the polymer matrix and nanoparticles. While results of optical properties for ($PS/SiC/Sb_2O_3$)nanocomposite showed that the absorbance, absorption coefficient, extinction coefficient, refractive index, real and imaginary dielectric constants, as well as optical conductivity increases with an increase in the concentrations of SiC and Sb_2O_3 nanoparticles, while the energy gap and transmittance decrease with increasing concentrations of nanoparticles. The results of electrical properties of nanocomposites showed that the dielectric constant and dielectric loss increase with increasing concentrations of nanoparticles and decrease with increasing frequency of applied electric field. While the A.C electrical conductivity increases with increasing the frequency and weight concentrations of (SiC/Sb_2O_3) nanoparticles. The results of applications of ($PS/SiC/Sb_2O_3$) nanocomposites against bacteria showed that the inhibition zone diameter increases with increasing concentrations of nanoparticles

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Chapter Two : Theoretical Part

Chapter Three : Experimental Part

Chapter Four: Results, Discussion and Future Work

List of Symbols

Symbols	Physical Meanings
n	Refractive Index
K	Wave Vector
A	Absorptance
I_O	Incident Intensity of Light
I_A	Intensity of absorbed light
I_T	The Intensity of Transmittance Ray
T	Transmittance
α	Absorption Coefficient
h	Plank Constant
v	Velocity of Light
E_g	Energy Gap
B	Constant Depended on the Type of Material
E_{Ph}	Energy of Photon

t	***Thickness***
λ	***Wavelength of Light***
c	***Velocity of Light***
k	***Extinction Coefficient***
i	***Imaginary Number***
R	***Reflectance***
ε_1	***Real Dielectric Constant***
ε_2	***Imaginary Dielectric constant***
N	***Complex Refractive Index***
σ_{op}	***Optical Conductivity***
ε^*	***Complex Permittivity***
ε_o	***Vacuum Permittivity***
ε'	***Dielectric Constant***
C_P	***Capacitance in Parallel***
C_O	***Capacitance in Vacuum***
ε''	***Dielectric Loss***
D	***Dispersion Factor***
$\sigma_{A.C}$	***Alternating Current Conductivity***
ω	***Angular Frequency***
f	***Frequency***
μi	***Electrical Dipole Moment***
P	***Polarization***
N_O	***Number of Molecules Per a Unit of Volume***

List of Abbreviations

Symbol	***Physical meaning***
C.B	***Conduction Band***
FE-SEM	***Field Emission Scanning Electron Microscope***
FTIR	***Fourier Transformation Infrared Ray***
OM	***Optical Microscope***
Ps	***polystyrene***
SiC	***Silicon Carbide***
Sb_2O_3	***Antimony Trioxide***
V.B	***Valance Band***
NPs	***Nanoparticles***
NCs	***Nanocomposite***

List of Tables

1.1 Introduction

Nanotechnology is a fast evolving multidisciplinary technology that has risen in popularity in a variety of domains in the last 10 years, including materials sciences, mechanics, electronics, optics, medicine, and biotechnology Airspace and oil. Its societal impact has been recognized as a crucial trigger. The prefix "Nano" is derived from the Greek word for "dwarf". The term "Nano" refers to anything incredibly tiny. A nanometer (nm) is one billionth of a meter and equals 10 angstroms. As example, a nanometer is 10^{-9} meter in length and 10000 times smaller in diameter than the diameter of a human hair [1] Nanotechnology will enable the improvement of innovative materials, laying the groundwork for the creation and improvement of unique features and structures, resulting in greater performance, lower maintenance costs, and enhanced usefulness[2] Nanotechnology applications have only grown in recent years, with materials holding the most promise, followed by electronics and medical. The following are some examples of probable nanotechnology uses[3]

-Miniature photovoltaic solar thin film cells for efficient energy generation in a variety of applications such as cellphones and autos

-Barriers for thermal and optical application

-Structural and electronic nanocomposite polymers and thin protective coverings.

-Semiconductors and microprocessors are faster, smaller and more powerful

- Ultra-light weight, high strength, precision formed materials

Nanotechnology is defined as the power, by operating at the molecular level atom by atom to build vast structures with essentially new functional properties. Nanotechnology is characterized as the production and control of nanomaterials matter with extreme precision[4] Composite materials are engineering materials that are the combination of at least two or more components(mixed and bonded) with distinct boundaries between them Components do not dissolve or merge completely into one another. Furthermore fillers and reinforcements are a good solution in order to reinforce the different physical or/and chemical properties and make these materials stronger together than would each individual material. The combination of different materials allows for the creation of a completely new composite material with a wide range of functional properties: mechanical, chemical, electrical, magnetic, optical and many others. Composite materials comprised metallic or non-metallic (polymer, ceramic, etc.) matrix and reinforcement – fibers, powders etc. – that is specifically distributed in the matrix. Depending on the used matrix materials exist three main sorts of composite materials such as: MMCs (Metal Matrix Composites), CMCs (Ceramic Matrix Composites)and PMCs (Polymeric Matrix Composites)[5] In recent years the bulk of polymers were only used in the manufacturing of low-cost, low-functioning goods[6] Polymer materials represent ∼20%, by weight, of electrical and electronic equipment by offering comprehensive properties that no other class of materials can give however, the continued miniaturization of electronic device components is coupled with the requirements of heat dissipation and fire safety, which requires improved thermal conductivity and enhanced flame retardancy of polymer materials[6]

1.2Composite Materials

Composite materials are a system of materials consisting of a mixture of two or more materials differing in the material's form or structure, and the properties of a composite differ from those of a material[7] The composite is made up of two main components: the matrix (basic material) and the additives. The matrix encloses and forms the composite, and the additives encircle and make the other components more cohesive in "compact structure" forming. Additives are components added to polymers which give them certain characteristics and improve basic characteristics. These components can improve overall conductivity, reduce porosity, increase friction, and improve some magnetic properties, and other things[8]

1.3 Polymer Structure

The physical properties of polymer materials depend on the molecular weight and the shape of it as well as on the molecular structure[9] a polymer consists of organic molecules (macromolecules) of small repeating structural units (monomers) connected to each other by a special 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[10]

1.4 Classification of Polymers

1.4.1Thermal Classification of Polymers

Polymers can be classified into two groups according to the effect of temperature on them.

a. Thermoplastic Polymers: The effect of temperature on these polymers affects their properties. As the temperature increases, the polymers be sticky and flexible; polymers return to their solid state if the temperature decreases. This is due to the thermoplastic polymer's molecules being held together by Intermolecular powers are relatively weak (Van der Waals forces). These molecules, including polystyrene, polyethylene, polypropylene, and polyvinyl chloride, slip over each other when heated[11,12] as figure(1.1) shows the atomic configuration of thermoplastic polymer

Figure (1.1) shows the atomic configuration of thermoplastic polymer [12]

b. Thermoset Polymers: Thermoset is a class of polymer obtained from curing or cross-linking of thermosetting resin or prepolymer using heat or radiation energy in the presence of hardener or cross-linking agent along with an initiator with or without the use of catalysts. The curing of prepolymers resulted in the formation of an infusible and insoluble high-molecular-weight solid mass with a three-dimensional network structure through the cross-linking of macromolecular chains. These polymers cannot be remitted or reshaped once cured due to the formation of an irreversible chemical bond. Thermosets have outstanding resistance toward heat, solvents, and mechanical deformations. Also, these materials offer good strength and modulus, high dimensional stability, and excellent stress cracking resistance [13]

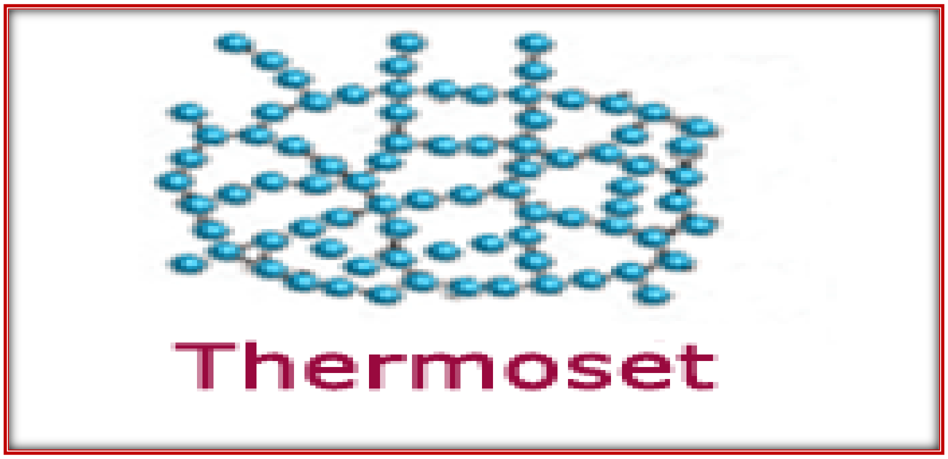


Figure (1.2) atomic configuration of thermosetting Polymers[13]

1.4.2Classification of Polymers According to Source

a. Natural polymer: Natural polymers by themselves are a class of polymers which refer to polymers sourced from nature (plants or animals). They include mainly carbohydrates and proteins which exist in plants and animals providing mainly structural support. This refers to polymers that are derived through extraction from their bulk form in nature, for example, cellulose or lignin extracted from wood. This also includes polymers produced by biological process such as bacteria synthesis or fermentation[14]

b. Synthetic Polymers: Polymer made of simple chemical compounds that constitutes the most important industrial polymers, including plastics, synthetic leather, nylon materials and a number of other c types. Synthetic polymers provide some other properties such as mechanical and physical properties and thermal stability[14,15]

1.4.3Classification of polymers according to homogeneity

Polymers are classified according to the homogeneity of the repeater unit into.[16]

a. Homo polymers

If the building blocks of the polymer are of the same kind as in poly therphethal ethylene.

b. Copolymers. When the building blocks of a polymer are more than one type, as in the polymer (styrene – butadiene).

c. Composite Polymers: are polymers prepared by adding additives to a homogeneous polymers matrix in order to improve or create new properties[17,18]

1.5 Nanocomposites

Nanocomposites can be defined as substances that appear at least one dimension in the nanometer range", and the size of the addition to the nano-miter, and the interactions become highly significant and result in significant changes in the properties of the final material. The nanocomposite consists of two parts, "filler and matrix", a traditional material in addition to padding is a nanomaterial[19,20] Nanocomposite materials have emerged as suitable alternatives to overcome limitations of micro composites and monolithic, while posing preparation challenges related to the control of elemental composition and stoichiometry in the nanocluster [21] Due to its expected remarkable thermal, optical, electrical, and antibacterial capabilities, polymer-based nanocomposites have received a lot of attention. Inorganic materials are favored because of their great thermal stability, good electrical characteristics, and high refractive index. However, research has indicated that inorganic nanoparticles cannot effectively serve a variety of industrial device applications due to a number of limitations[22]

1.6 Polymer Nanocomposites

Polymer nanocomposites have been proposed or are being used for numerous applications, ranging from car bumpers to advanced optoelectronic devices. Understanding the impact of Nano fillers on the composite mechanical properties is critical to the success of all of these applications. Consequently, a large number of research groups are focused on developing a general framework for predicting, or at least, understanding how the chemistry and morphology of the polymer matrix synergizes with the surface chemistry, the size, and the shape of a nanoscale filler to define mechanical properties. Within this general framework, the underlying mechanisms lie at the intersection of chemistry, physics, materials science, and continuum mechanics. Therefore, the researchers involved in this critical area of science have an equally varied assortment of backgrounds and approaches[22,23]

1.7 Applications of Polymer Nanocomposites

Polymer nanocomposites have gotten a lot of attention in academia and industry over the last few decades and they've become a key component in the development of novel advanced materials for a variety of applications [24]

-Cars (gasoline tanks, fenders, interior and exterior panels...etc)

- Construction (pull out the shape and panels)

- Electronics and electricity (printed circuits and electrical components).

- Food packaging (packaging, films)

- Cosmetics (controlled release of active ingredients)

- Dentistry (filling materials)

1.8 Polystyrene

Polystyrene (PS) is an amorphous polymer with bulky side groups General properties of PS are hard, rigid, and transparent at room temperature and glass like thermoplastic material which can be softened and distort under heat. It is soluble in aromatic hydrocarbon solvents, cyclohexane and chlorinated hydrocarbons. Polystyrene was first produced commercially in late 1930. Polystyrene made from the aromatic monomer styrene as its basic unit. Polystyrene is one of the most widely used kinds of plastics Polystyrene is commercially manufactured from styrene which is prepared from benzene and ethylene under pressure and uses of Aluminum Chloride as a catalyst[25] Polystyrene (PS) composites including nanocomposites have gained wide applications in different branches of industry because of their low cost, low density, chemical inertia, and low thermal conductivity. However, the dielectric constant and thermal conductivity of PS is very low. In some applications especially as electrical and electronic packaging materials, high thermal conductivity is needed to dissipate heat, and maintain operating temperature[26] Table (1.1) properties of polystyrene (PS)

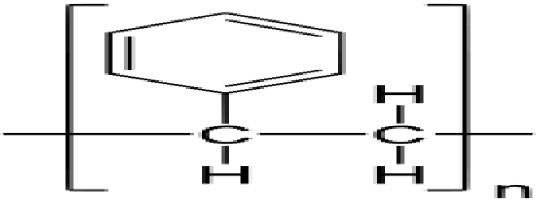


Figure (1.3): Molecular formula of PS [26]

1.9 Silicon Carbide (SiC)

Silicon carbide (SiC) is a nonoxide semiconductor ceramic material with many excellent properties, such as high thermal conductivity, passivity to reactions with acids and melts, superb oxidation resistance, excellent thermal shock resistance, and extremely high hardness, which make it widely used in microwave dielectrics and the power energy storage materials.[23,24] but the SiC nanoparticles are very easy to agglomerate which will influence the physicochemical properties of the composites[6] Due to its peculiar characteristics, SiC technology experimented with a high boost, attracting developments in new devices formulation. Besides its consolidated utilization as a bulk material, SiC also starts to be experimented as a filler in polymer matrices in the preparation of composite materials with the aim to enhance or improve selected properties[27,28,29] Silicon carbide has good physical properties as shown in (1-2) Table

1.10 Antimony Trioxide (Sb_2O_3)

Antimony trioxide (Sb_2O_3) is a semiconducting material and possesses excellent catalytic performance in photochemistry and superior chemical stability in flame retardance So far much attention has been focused on the synthesis of Sb_2O_3 films, and the exploration of their novel properties By comparison, low-dimensional Sb_2O_3, such as nanoparticles, nanowires, nanotubes, and nanoribbons, can be expected to exhibit special properties. It is well known that many of the properties of nano-scaled materials are shape-dependent therefore, controlled synthesis of desired morphologies of nanomaterials is exceedingly important. Although much effort has been invested in this direction, it is still a challenging task for the scientists to controllably synthesize a predetermined material morphology in a facile way[30,31] Antimony oxide (Sb_2O_3) has wide applications as effective catalyst, retardant, conductive materials, functional filler and optical materials. In addition, Sb2O3 is very useful as conductive materials, high-efficiency flame-retardant synergist in plastics, paints, adhesives and textile back coating[32,33]

1.11 Literature Review

Increased attention has been paid in recent years to research on polymer composites in general and nanocomposites in particular, from the point of view of their potential uses in mechanical, optical, electrical and thermal applications a brief summary of recent developments in the abovementioned fields is given below

In(2013) **T. Tsuruoka** *et a*l[34] studied the optical properties of PS/ Au nanocomposite films. He found the absorption coefficient increases with increasing of the filler wt % content. The forbidden energy gap decreases with increasing of the wt % filler.

In(2014) **X.Yan** *et al* [35] prepared PS/magnetite(Fe_3O_4) polymer nanocomposites (PNCs) are successfully synthesized by a solvent extraction method. Scanning electron microscopy (SEM) reveals that the nanoparticles are well distributed in the PS matrix with (5, 10, and 20)wt% without obvious agglomeration. Fourier transform infrared spectroscopy (FTIR) analysis indicated that the PS/Fe_3O_4 PNCs are synthesized with strong interaction between PS and (Fe_3O_4) nanoparticles.

In (2015) **Y. Kumari**, *et al* [36] studied the structural and morphological properties of PS/TiO_2 nanocomposites were investigated by optical microscopy(om), they found that result of The Optical microscop (OM) revealed that TiO2 nanoparticles were distributed in the PS film inhomogenously and the particles were agglomerated Agglomeration becomes more intensified in the films with higher concentration of TiO_2 .

In(2016) **A. M. Nuruzatulifah** *et al* [37] studied the synthesis and characterization of polystyrene nanoparticles with covalently attached fluorescent dye.The morphology and functional group identification was characterized using Scanning Electron Microscope (SEM) and Fourier Transform Infra-red (FTIR), respectively. As a result, SEM images showed that synthesized polystyrene particles were spherical in shape. The size of polystyrene particle was ranging between 40 – 60 nm and a slight growth of the particles size was observed after the encapsulation of dye which ranges 60 - 70 nm.

In(2017) **S. Bhavsar**, *et al* [38] simple solution casting method was utilized to synthesize aluminium oxide (Al_2O_3)doped polystyrene (PS) polymer nanocomposite films. As synthesized films were characterized using Fourier transform infrared (FTIR)spectroscopy, and scanning electron microscopy (SEM).A new carbonyl group appeared in the FTIR spectra and confirmed the charge transfer reaction between filler and polymer matrix. SEM analysis indicates the agglomeration of Al2O3 nanoparticles into PS matrix at higher concentration

In(2018) **B. Demirbay and Ş. Uğur** [39] studied the electrical and morphological properties of nanocomposite films made up of polystyrene (PS) latex which have different particle sizes and multi-walled carbon nanotubes (MWCNTs) were reported. Increment in PS latex size lead to the increase in the conductivity one order of magnitude from 10^{-5} S for 382 nm latex systems to 10^{-4} S for 560 nm latex system. The addition of MWCNTs as a nanofiller into PS latex enhanced the conductivity by 9 and 10 orders of magnitude, from 10^{-15}-10^{-13} S for the pure PS polymers to 10^{-5}-10^{-4} S at 20 wt% of MWCNTs. SEM images also showed the improved MWCNT dispersion, with the increase in latex particle size in consistent with these experimental results

In(2019) **S. S. Manhas**, *et al* [40] studied the effect of the nanocomposite containing polypyrrole and polystyrene synthesized by solution cast technique. The effect of different (especially small) concentrations of polypyrrole on structural and optical properties was studied. The results revels that properties can be tuned significantly even with inclusion of small filler concentration in the polymer matrix.A drastic decrease in the transmittance (up to 35%) has been observed even with small amount of filler concentration (i.e. 3%)

In (2020) **N.Narang and A.K.Tyagi** [41] studied the Core-shell structured nanoparticles of PS- ZnO were successfully synthesized in PS matrix by wet chemical method and transparent thin films of these nano-hybrids were coated on substrates by using spin coating technique. Structural and optical properties of all the nanocomposites samples were investigated by XRD, FTIR and UV-Visible spectroscopy.

In(2021) **S. S. Bag**, *et al* [42] studied The addition of nanoparticles such as silver nanoparticles (AgNPs) into PS enhances its mechanical properties, gas barrier properties, thermal stability, and so forth. This study reports the development of PS/Ag nanocomposite using green synthesized Ag NPs and waste thermocol, the green synthesized AgNPs were prepared in different concentrations and embedded accordingly into the PS matrix. The morphology of PS/Ag NCs was studied using

Field Emission Transmission Scanning Microscopy (FE-SEM) and Fourier transform infrared spectroscopy (FTIR) was used to evaluate the prepared nanocomposites' surface chemical bonding and surface composition. . These PS/Ag NCs showed an antibacterial effect against Escherichia coli, a disease-causing gram-negative bacteria commonly found in water. Among them, the PS/Ag NCs cup encapsulating 10% AgNPs showed optimum tensile strength and bacteria disinfection property. These nanocomposites have been utilized to prepare cups as a model of water tank for water storage having disinfection properties.

In(2022) **U. Kumar** *et al* [43] studied the of effcet europium-doped barium titanate particles were used as filler material and polystyrene was used as a matrix to fabricate PS/Ba1−3x/2EuxTiO_3/nanocomposites with x = 0, 0.005, 0.015 and 0.025. A solid-state reaction was used to synthesize filler particles and . The effects of ultrasonic treatment were also studied in the formation of nanocomposite materials. The quantitative and qualitative studies were conducted using X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR), field emission scanning electron microscopy (FE-SEM), and ultraviolet-visible(UV-Vis) characterization techniques. The XRD data and FTIR data confirm the incorporation of filler particles in the polymer matrix. FE-SEM data confirms that the particles are in the nanophase.The optical band gap was directly affected by the filler particles and it started to reduce as concentration started to increase.

1.12 The Aims of Work

1- Preparation of (PS/SiC/ Sb_2O_3) nanocomposites

2- Studying the structural, optical and electrical properties of (PS/SiC/Sb_2O_3) nanocomposites

3- Test the antibacterial application of PS/SiC/Sb_2O_3 nanocomposites

Chapter Two
Theoretical Part

2.1 Introduction

This chapter has a theoretical explanation (the theoretical part). It concentrates on theories of optical characteristics, in particular absorption, polarization, and electrical properties. The enhancement of optical and electrical characteristics in particular has led to an increase in research into nanocomposites. Due to their desirable electrical characteristics and high refractive index, nanoparticles serve as sophisticated technological materials.

2.2 Optical Properties

The changes in electrons properties with size result in major changes in the optical Properties of nano sized materials. As particles are rendered small enough, quantum effects occur, limiting the energies at which electrons and holes can reside in the particles, since energy is proportional to wavelength. This means that the particle's optical properties can be fine-tuned depending on its size. Particles may thus be made to emit or absorb particular wavelengths of light simply by changing their size Knowing the absorption and transmission spectrum of a polymer helps to distinguish certain optical characteristics of various wavelength ranges. A UV test allows us to know the form of the links, the orbital beams and the energy beams. The analysis of the spectrum range of visible applications provides ample information on solar application activity. In order to know the overall structure of a polymer and its chemical structure, the analysis of the infrared range is necessary[44,45]

2.2.1 Absorbance

Absorptance can be defined as the ratio between absorbed light intensity (I_A) by material and the incident intensity of incident light (Io) and the absorbance is a unit-free quantity. It is given by the following relationship[46]

$$A=I_A/I_o \tag{2.1}$$

2.2.2 Transmittance

It is defined as the ratio between the intensity of the radiation flowing through the membrane (I_T) and the original intensity of the radiation incident on it (Io), which is also a quantity devoid of units, and is given by the following relationship[47,48]

$$T = I_T / I_o \tag{2.2}$$

2.2.3 Fundamental Absorption Edge

The fundamental absorption edge is characterized as the rapid increase in absorption if the energy radiation absorbed is almost equal to the energy gap in the bands. Thus, the essential absorption edge represents the less energy difference between the top and the bottom of the conduction bands [49] the regions of absorption can be divided into three distinct regions

a) High absorption region**.**

figure (2.1) shows this area. The absorbent coefficient magnitude (α) in section (A) is greater or equal to (10^4 cm^{-1}). This could include a forbidden optical energy gap.

b) Exponential region: the value of absorption coefficient (α) is ($1cm^{-1} <\alpha< 10^4 cm^1$).

c) Low absorption region: As shown in Figure (2.1), which depicts the absorption zones, the absorption coefficient (α) is very small, measuring just approximately ($1cm^{-1}$).

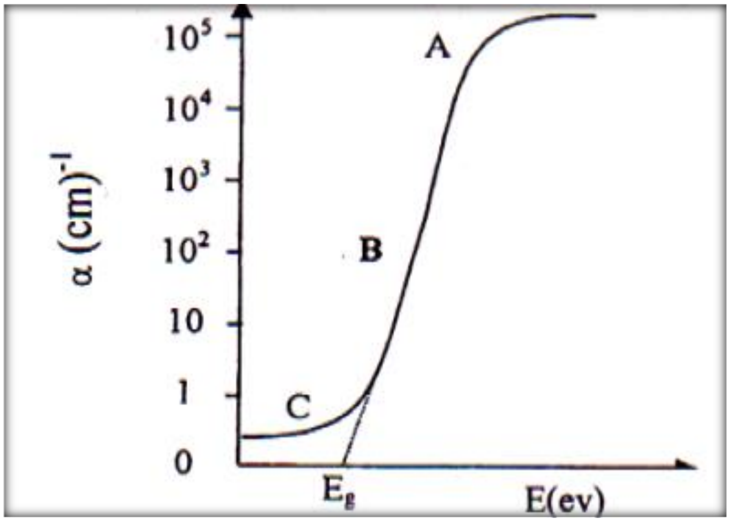


Figure (2.1) the absorption regions [49]

2.2.4 The electronic transitions

There are two basic types of electronic transition ,direct and indirect transition[50]

1- Direct Transition

This transition happens in semiconductors when the bottom of the 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 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[51] These direct transitions have two types[52]

a) Direct Allowed Transition

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

b) Forbidden Direct Transition

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

The absorption coefficient for this transition type is given by [53]

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

Where: $E_{opt.}$ energy gap between direct transitions.

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 the curve (E-K), in these transitions the bottom (C.B.) is not above the top of (V.B.) The electron transits between (V.B.) and (C.B.) are not perpendicular if the magnitude of the electron's wave vector is not identical before and after transfer ($\Delta K \neq 0$). This kind of transformation occurs with the beneficial "Phonon" particle for energy conservation and energy law, two kinds of indirect transitions exist[54,50]

a) Permitted indirect transitions

These transitions happen between the top of (V.B) and the bottom of (C.B) 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 at the top of (V.B) and near points in the bottom of (C.B), as shown in Figure (2.2-d).

The absorption coefficient for transition with a phonon absorption is given by [55]

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

Where: E_{ph}: Phonon energy: (-) is absorbed by phonon, and (+) is emitted by phonon

(r = 2) for the indirect transformation permitted, (r = 3) for the indirect transformation that was prohibited.

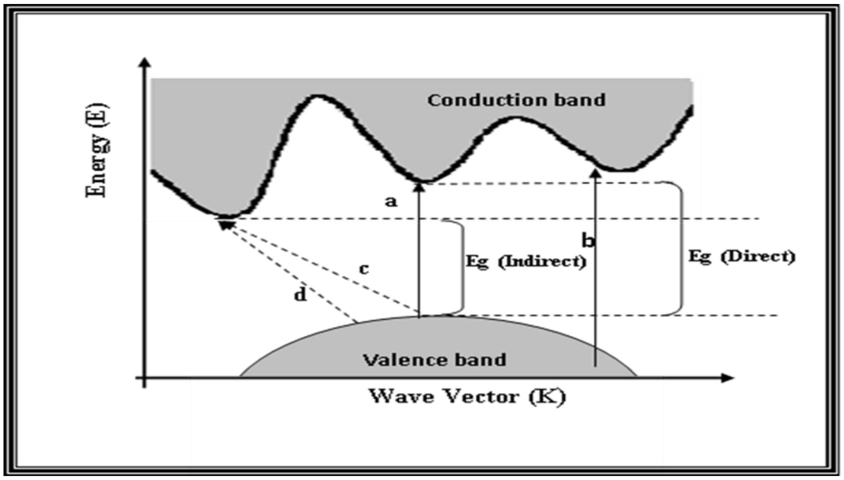


Figure (2.2) the transition types [55]

(a) allowed direct transition **(c) allowed indirect transition**

(b) forbidden direct transfers **(d) forbidden indirect transition**

2.2.5 Optical Constants

2.2.5.1 Optical absorption coefficient (α)

Is defined in the direction of wave diffusion in the medium as the progressive decrease of incident energy flow in an incident field. The coefficient of absorption is affected by photon energy and semiconductor features such as gap energy and electronic transitions[56,57] The following equation defines the connection between incident (I_o) and penetrating (I) light absorption.

$$I= I_o\, e^{-\alpha t} \qquad (2.5)$$

Where (t) is the matter thickness (α) is the absorption coefficient measure in cm^{-1}

$$e^{\alpha t} =(I_o/I) \qquad (2.6)$$

$$\alpha t=\log(I_o/I)^{A} \qquad (2.7)$$

Where log I/I_o is the absorbing number (A), this is the way to measure the absorption coefficient[58]

2.2.5.2Extinction coefficient (k)

It is defined as the amount of attenuation in the intensity of electromagnetic radiation caused by the interaction between electromagnetic rays and particles of the thin film material. The damping coefficient may be computed using the following equation, which is connected to the absorption coefficient[59]

$$k = \alpha\lambda /4 \pi \qquad (2.8)$$

Where λ (cm) is the wavelength of the incident radiation and α (cm^{-1}) absorption

Coefficient

2.2.5.3Refractive index (n)

The index of refraction of a material is the ratio of the velocity of the light in vacuum to that of the specimen[60]

$$n=c/v \tag{2.9}$$

where (n) refractive index, (c) the velocity of light in a vacuum, and (v) the velocity of light in any material medium[61,62]

$$N = n + ik \tag{2.10}$$

Where: N is the complex refractive index, n is the real part of refractive index and K is imaginary part of the refractive index (extinction coefficient)

The relation between absorption coefficient and the molar absorptivity or extinction coefficient (k) is

$$k = \frac{\alpha\lambda}{4\pi} \tag{2.11}$$

Where (λ) the wavelength, the real part of refractive index (n) can be determined by

$$n= \frac{1+\sqrt{R}}{1-\sqrt{R}} \tag{2.12}$$

Where (R) is the reflectance

2.2.5.4 Dielectric Constant (ε)

The dielectric constant reflects a matter's ability to polarize, allowing it to react in a complex way to different frequencies. The electronic polarity dominates the other forms of polarization at optical frequencies that are expressed by light waves [63] by the following equation, the real and imaginary dielectric constant can be determined [64]

$$\varepsilon = \varepsilon_1 - \varepsilon_2 \qquad (2.13)$$

Where ε: complex dielectric constant, ε_1 :the real part of the dielectric constant, and ε_2 : the imaginary part of the dielectric determined constant. The real and imaginary part of dielectric constant can be by using equations[65]

$$\mathcal{E} = N^2 \qquad (2.14)$$

$$n = (n + ik_o) = \varepsilon_1 + i\,\varepsilon_2 \qquad (2.15)$$

From equation (2.13) real and imaginary complex dielectric coefficient can be written as follows

$$\varepsilon_1 = (n^2 - k_o^2) \qquad (2.16)$$

$$\varepsilon_2 = (2nk_o) \qquad (2.17)$$

2.2.5.5 Optical Conductivity (σ_{op})

Is the phenomenon of an increase in the number of charge carriers (electrons or holes) as a result of a light beam incident on a semiconductor, the optical conductivity (σ_{op}) depends directing on the refractive index (n) and absorption coefficient (α) the optical conductivity can be calculated from the equation[66,67]

$$\sigma = \frac{\alpha n c}{4\pi} \qquad (2.18)$$

Where (σ_{op}) is the optical conductivity, (α) is the absorption coefficient, (n) the refractive index, (c) the velocity of light

2.3 Electrical Properties.

Polymers are generally insulators, but they are also not completely free of conduction mechanisms. Conduction often occurs due to impurities that include concentrations of charge carriers[68] Insulators can be used to store electrical energy in the form of charge separation when the electron distributions around the constituent atoms or molecules are polarized by an external electric field[69]

2.3.1 The A.C electrical conductivity

The electric field frequency in the A.C conductivity would be variable during Dielectric materials can be used to store electrical energy by separating the charge by applying an external electric field. So, when applied a low-frequency electric field on the insulator the permanent or induced dipoles keep pace with the direction of the applied electric field, that is, the material becomes polarized[70,71] The complex permittivity of a material (ε^*) can be written as[72]

$$\varepsilon^*=\varepsilon_1+i\varepsilon_2 \qquad (2.19)$$

Where ε_1 and ε_2 are value real and the imaginary parts of complex permittivity and Permittivity and imaginary number equal $\sqrt{-1}$. The real part is determined by [73]

$$\varepsilon_1 = \varepsilon_o \varepsilon' \qquad (2.20)$$

The magnitudes of ε_1 and ε_2 depend on the angular frequency (ω) of applied the electric field. The magnitude of ε_o (or the dielectric constant ε') indicates the ability of material to store energy from applied electric field[74] The equation can be used to measure the capacitance of a capacitor made up of two parallel plates[73]

$$C = \varepsilon' \varepsilon_o A/t \qquad (2.21)$$

Where ε' is the dielectric of constant, t is the sample thickness and ε_o is Permittivity in vacuum. Dielectric constant is given by the relation[75]

$$\varepsilon' = C_P / C_O \tag{2.22}$$

Where: C_P is capacitance in parallel and C_o this is vacuum capacitor [74] the dielectric of loss (ε") is given by

$$\varepsilon'' = \varepsilon' D \tag{2.23}$$

Where D is dispersion factor, and this measures the lost electrical energy in the sample from the applied field which is transformed to thermal energy in the sample. The dissipated power in the insulator is represented by the existence of alternating potential as a function of the alternating conductivity is given by [75]

$$\sigma_{A.C} = \omega\varepsilon_o \varepsilon' \tag{2.24}$$

Where ωis an angular frequency ($\omega = 2\pi f$)

2.3.2 The Electrical Polarization

When the condenser terminals consisting of an electric insulator between their plates are electrically moved, local displacements occur in positive and adverse charging centers, resulting in an electric polarity operation. Its value is the number of all dipoles in the unit volume of the sample[76]

$$\mu i = p\,E^{-}\mathrm{i} \tag{2.25}$$

Where μi is the electric dipole moment, p is the atom or molecule's polarity and Ei^{-} is a molecule internal field, proportional to the external field. Thus, for the unit length, the complete dipole moment (P):

$$P = N_{\circ}\mu i \qquad (2.26)$$

Where, N_o the volume unit is the number of molecules. Electrical polarization takes place in all insulators due to the negative or positive charging of the impurities, electrons, molecules and ions. The following equation is able to express the electrical polarization resulting from electrical field effect [77]

$$P= D- \varepsilon_o E \qquad (2.27)$$

Where D is the electric change, E is the strength of electric field and ε_o is free space permittivity or permittivity to vacuum (8.85×10-12 F/m)

$$D= P+ \varepsilon_o E= \varepsilon_o \varepsilon' E \quad (2.28)$$

As

$$\because \varepsilon'= D/\varepsilon_o E \qquad (2.29)$$

Then,

$$\therefore \varepsilon'=1+\frac{p}{\varepsilon o E} \qquad (2.30)$$

Where ε' Dielectric constant.

The balance of a volume unit's relative dielectric constant and polarity indicates the connection with Clauses- Mossotti [78]

$$\frac{N_{\circ}P}{3\varepsilon_{\circ}}=\frac{\acute{\varepsilon}-1}{\acute{\varepsilon}+2} \qquad (2.31)$$

This equation can be applied to the electric insulators ionic and nonpolar.

2.3.2.1 Mechanism of Polarization

The components of the polarization can be defined by polarizing of substances to demonstrate the form of total polarization figure (2.3) Polarization mechanism [78]

$$P_{total} = P_e + P_d + P_o + P_i \qquad (2.32)$$

A- Electronic Polarization (pe)

The charge distribution is distorted by an external electrical field as shown in figure (2.3-a) this occurs because of the nucleus positive charge and the negative charge center are separated and induced dipoles are produced It happens very quickly (10^{-15}seconds) and is temperature independent. This kind of polarization is also called optical polarization [79]

B- Ionic Polarization (Pi)

Ionic bonding materials can be ionic polarized. Ion polarization is the shift in positive and negative electrodes, as seen in the figure (2.3-b), since only when an external electrical area is available is the relative movement of positive and negative ions. For ion polarization to be set, it takes a short time, but longer than for electronic polarization [79]

C- Rotational or orientation polarization (P_d)

It occurs with the permanent dipole moment of molecules. The dipole rolls around the axis when applied to an electric field and arranges in the direction of the field. This type of polarization is temperature dependent and takes a long time[80],like in figure (2.3-c)

D- Interfacial polarization, also known as space charge (P_0)

When a problem involves impurities, vacuum, or structural defects, the opposite charge is concentrated at the impurity terminal, The balance of a volume unit's relative dielectric constant and polarity indicates According to the defect that causes polarization, The bulk of it exists in radio waves which can exceed frequencies lower than those of human hearing.as shown in figure (2.3-d) [81]

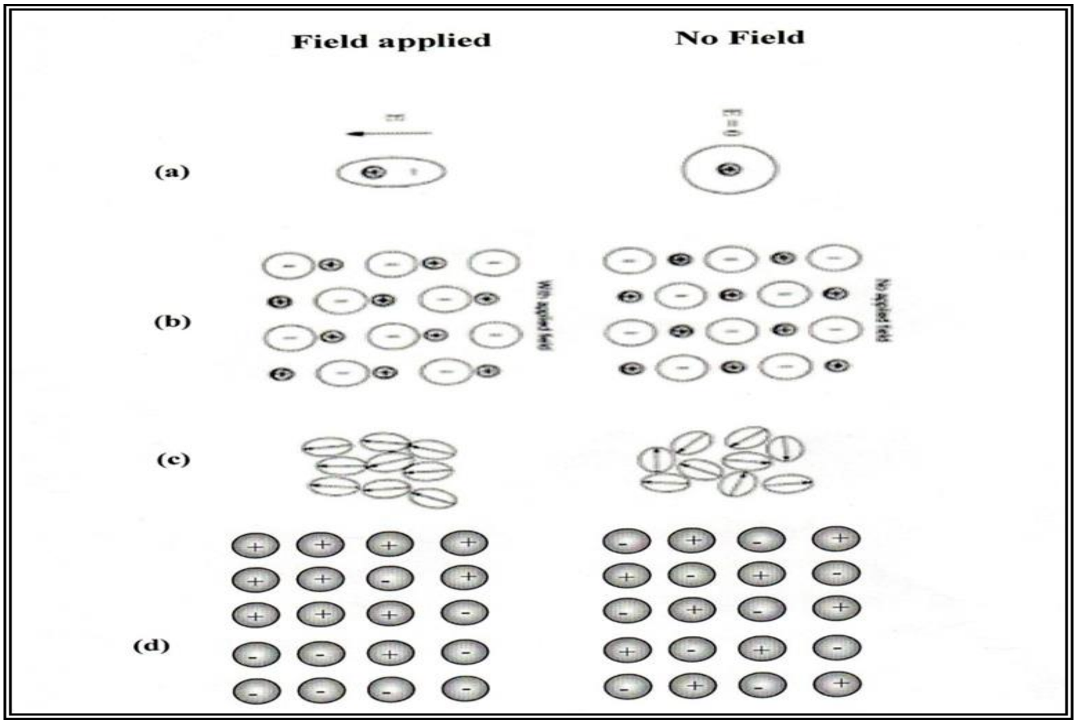


Figure (2.3) the four types of polarization [81]

a- Electronic polarization b- Ionic polarization

c- Orientation polarization d-Space charge polarization

2.4 Antibacterial Activity

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[82] 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[83]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[84] 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[85,86] Figure (2.3) show mechanisms for antibacterial activity of nanoparticles

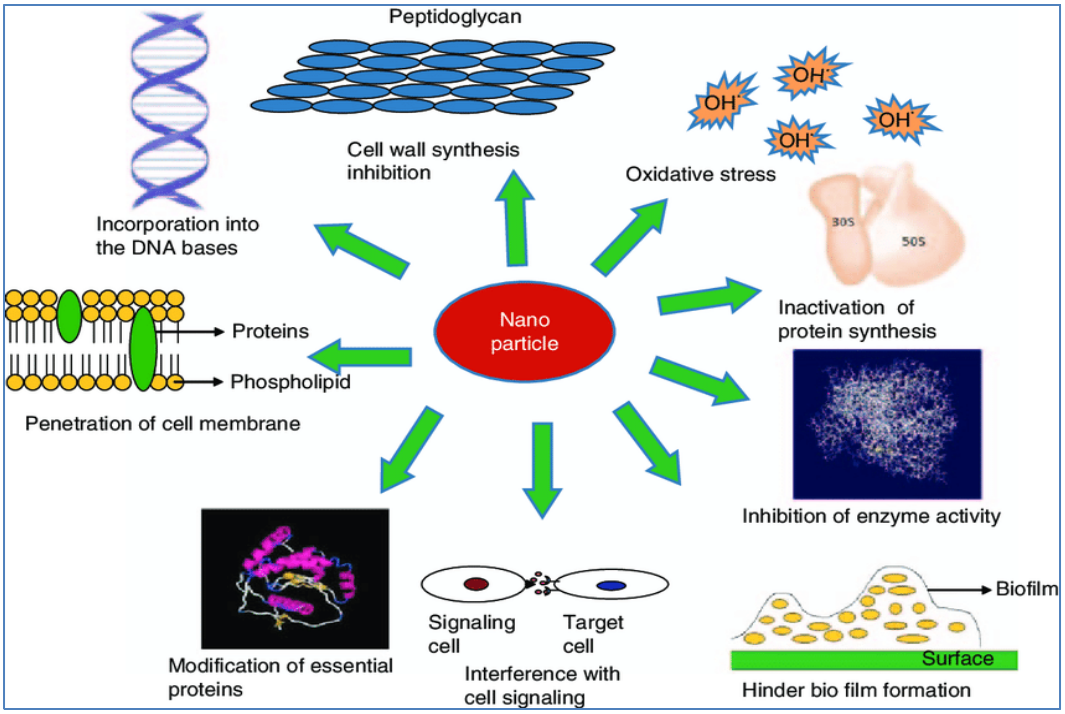


Figure (2.4) Mechanisms for antibacterial activity of nanoparticles [86]

Chapter Three

Practical Part

3.1 Introduction

This chapter includes the preparation process, devices and measurement techniques. A general description of materials (polystyrene, silicon carbide, antimony trioxide) used in this work are given by (optical microscopic, Fourier Transform Infrared Radiation (FTIR), Field Emission Scanning Electron Microscope (FE-SEM), optical properties measurements, measurement of A.C. electrical conductivity and includes diagrams some of electrical circuits, and measurements of antibacterial activity.

3.2 The Materials Used in This Work

3.2.1 Polystyrene (PS)

Itis a chemical compound that is a synthetic aromatic hydrocarbon polymer polystyrene is one of the most widely used plastics around the world, with an estimated production volume of several million tons annually used as granular form and could be obtained from local markets high purity (99.97%). Table (3.1) properties of polystyrene (PS)

Figure (3.1) Polystyrene (PS) polymer

Table (3.1) properties of polystyrene (PS)

Chemical formula	$(C_8H_8)_n$
Class	100C^o
Density	10.5g/cm^3
Melting point	239C^o
Its absorption of water	0.05%
refractive index	1.59~1.6

3.2.2 Silicon Carbide (SiC)

It is a chemical compound of silicon and carbon, with the symbol SiC, and it exists under standard conditions as a dark-colored crystalline solid.it was obtained as powder from US Research Nanomaterials, Inc, USA with size (<80nm, cubic) and high purity (99%). Table (1.1) properties of polystyrene (SiC)

Figure (3.2) Silicon Carbide nanoparticles

Table (3-2). Physical properties of silicon carbide (SiC)

Properties	Silicon Carbide SiC
Density	3.21 g/cm3
Melting Point	2730 C^0
Thermal Conductivity	3.6 W/cm.K
Crystal Structure	Cubic,cF8
Lattice Constant	4.3596 Å
Grain Size	80 nm
molecular weight	40.10
The appearance	Solid

3.2.3 Antimony Trioxide (Sb_2O_3)

It is a chemical compound with the formula Sb_2O_3, and it is in the form of a white crystalline powder. Antimony trioxide belongs to the group of inorganic flame retardants. It has a white or colorless color depending on its internal structure, where the cubic structure is colorless, while the rhombic structure is white. Antimony oxide (Sb_2O_3) has good physical properties as shown in (2-2) Table

Figure (3.3) Antimony Trioxide Nanoparticles

Table (3-3). Physical properties of Antimony oxide (Sb_2O_3)

Properties	**Antimony oxide (Sb_2O_3)**
Density	5.2 g/cm3
Melting Point	656 C^0
Moller mass	291.52g/mol
boiling point	1425C^0
The appearance	White crystalline powder

3.3 Preparation of ($PS/SiC/Sb_2O_3$) Nanocomposites

In order to make ($PS/SiC/Sb_2O_3$) nanocomposites, 1 gm of polystyrene (PS) was dissolved in 30 ml of chloroform, and the polymers were then stirred for 30 minutes at room temperature by using a magnetic stirrer. To make the solution more homogeneous, silicon carbide (SiC) and ternary antimony oxide (Sb_2O_3) nanoparticles were added at various concentration (0,2,4,6 and8) wt. %. After the solution was dried 1 days at room temperature, the ($PS/SiC/Sb_2O_3$) NCs were clipped off the petri dish has diameter of 10 cm.

3.4 Measurements of Structural Properties for($PS/SiC/Sb_2O_3$)NCs

3.4.1 Optical Microscope

The of ($PS/SiC/Sb_2O_3$) Nanocomposites are examined by using the optical microscope, which is supplied from Olympus name (Toup View) type (Nikon -73346) and equipped with light intensity automatic controlled camera. Under magnification (10x), this measurement was implemented in the University of Babylon /College of Education for Pure Sciences.

Figure (3.4) Optical Microscope used in the work

3.4.2Field Emission Scanning Electron Microscope

The surface morphology of (PS/SiC/Sb_2O_3) nanocomposites was tested for all samples by using scanning electron microscope. It is characterized by magnifying the image with a high accuracy of about 100,000 times, as a beam of electrons is directed to the surface and gives black and white images of the sample surface because it does not depend on light waves but on electronic emission, Were tested using a scanning electron microscope (Zeiss, Sigma, German origin) at Shahrud University of Technology, Iran

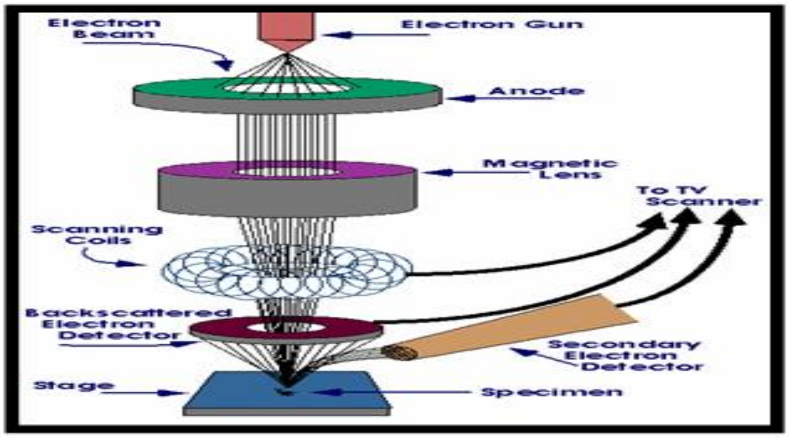


Figure (3.5) Set-up illustrates theFE- SEM

3.4.3 Fourier Transform Infrared Spectrometer (FTIR)

The Fourier Transform Infrared Spectrometer (FTIR) is a powerful tool for determining the types of chemical bonds. When infrared radiation is shined on a molecule, the molecule can absorb some of these waves and as a result gain energy and vibrate its atoms, resulting in an increase in the length of the bond (bond expands) i.e. a change occurred in the places of the atoms. The FTIR spectra of the ($PS/SiC/Sb_2O_3$) nanocomposites were recorded by FTIR (Bruker Corporation, German origin, type vertex-70) in the wavenumber range (1000-4000 cm^{-1}) at University of Babylon / College of Education for Pure Sciences / Department of Physics.

Figure (3.6) Fourier transform infrared spectroscopy device used in the work

3.5 Optical properties measurements

The Optical properties of the ($PS/SiC/Sb_2O_3$) nanocomposites films in the wavelength range (220-820)nm were recorded using a dual-beam spectrophotometer (SHIMADZO MODEL UV-1800 UVSPECTROPHOTOMETER) located at the University of Babylon/College of Education for Pure Sciences/Department of Physics. These measurements happened at room temperature.

Figure (3.7) Image of UV spectrophotometer (photometer).

3.6 Measurements of A.C Electrical Properties for NCs

The A.C electrical properties of (PS/SiC/Sb_2O_3) nanocomposites are measured by measuring the capacitance (Cp) and dispersal factor (D) using a type LCR meter (HIOKI 3532-50 LCR HI TESTER) using different frequencies of (100 Hz –5MHZ) at room temperature as shown in figure (3.8), in the College of Education for Pure Sciences, University of Babylon.

Figure (3.8) LCR hi tester device

3.7 Antibacterial Activity Application Measurements of NCs

The antibacterial activity of ($Ps/SiC/Sb_2O_3$) nanocomposites samples was tested by diffusion method. Antibacterial activities were carried out using Gram-positive (*Staphylococcus*) and Gram-negative (*Klebsiella*) organisms. Bacteria (*Staphylococcus* aureus and *Klebsilla*) were cultured in Muller-Hinton Medium. Discs ($PS/SiC/Sb_2O_3$) were placed on media and incubated at (37°C) for 24 hours. The diameter of the damping zone was measured.

Chapter Four

Results, Discussion and Future Work

4.1 Introduction

This chapter presents the findings and a discussion of the structural, optical; A.C electrical, and applications for antibacterial activity of (PS/SiC/Sb_2O_3) NCs

4 .2 Structural Properties of (PS/SiC/Sb_2O_3) Nanocomposites

4.2.1 The Optical Microscope (OM)

Figure. (4.1) Shows optical microscope images of PS/SiC/Sb_2O_3 nanocomposites with and without different concentrations of SiC and Sb_2O_3 NPs at magnification power (10x). Image, polystyrene (PS) is exceptionally miscible, as seen by its finer form and smooth, homogeneous surface, while in portraits b, c, d and e, it can be seen, that SiC and Sb_2O_3 NPs are well distributed on the surface of the polymer. from these images, the SiC and Sb_2O_3 NPs formed clusters in the form of chains that extended along the surface of the films, attributed to the novel property in SiC and Sb_2O_3 NPs[87] other than charge transport within polymer matrices, which also was enhanced by raising the percentages of SiC and Sb_2O_3 NPs

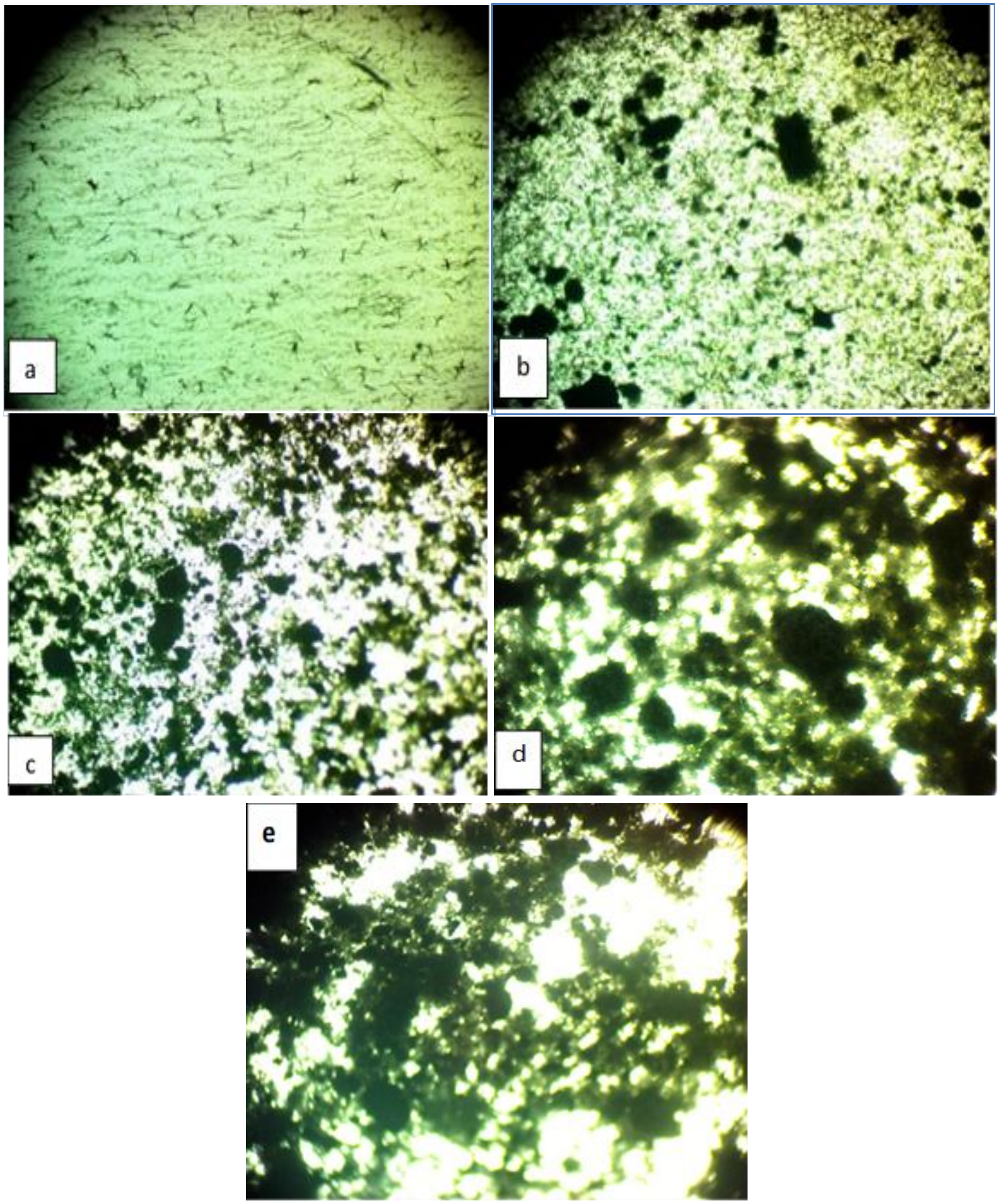


Figure (4.1) Photomicrographs (10X) for PS/SiC/ Sb_2O_3 nanocomposites (a) for (Ps) (b) for 2wt.% SiC/Sb_2O_3 nanoparticles, (c) 4wt.% SiC/Sb_2O_3 nanoparticles,(d) for 6wt.% SiC/Sb_2O_3 nanoparticles, (e) 8wt.% SiC/Sb_2O_3 nanoparticles

4.2.2 Field Emission Scanning Electron Microscope (FE-SEM) Of ($Ps/SiC/Sb_2O_3$) Nanocomposites

The dispersion of nanoparticles within the polymer is examined by FE-SEM, and the impact of the SiC/Sb_2O_3 nanoparticles on the nanocomposites is then confirmed. Figure (4.3) shows FE-SEM images of ($PS/SiC/Sb_2O_3$) nanocomposites with variable content of SiC/Sb_2O_3 NPs with a magnification (20 KX) Image (a) indicate that the polymer is homogenous, and cohesive it is evident the increase of SiC/Sb_2O_3 nanoparticles to ($PS/SiC/Sb_2O_3$) nanocomposites varies the scheme's surface profile (see images b, c, d and e). As explained in the images, the grain collections as the content of SiC/Sb_2O_3 NPs rises. The membranes' surface morphology ($PS/SiC/Sb_2O_3$) will be determined by the results. The amount of clusters or fragments that are dispersed on the upper surface of nanocomposites increases as the content of SiC/Sb_2O_3 NPs rises[88] the grain size of the ($PS/SiC/Sb_2O_3$) nanocomposites calculated from FE-SEM images, as shown in figure (4.2)

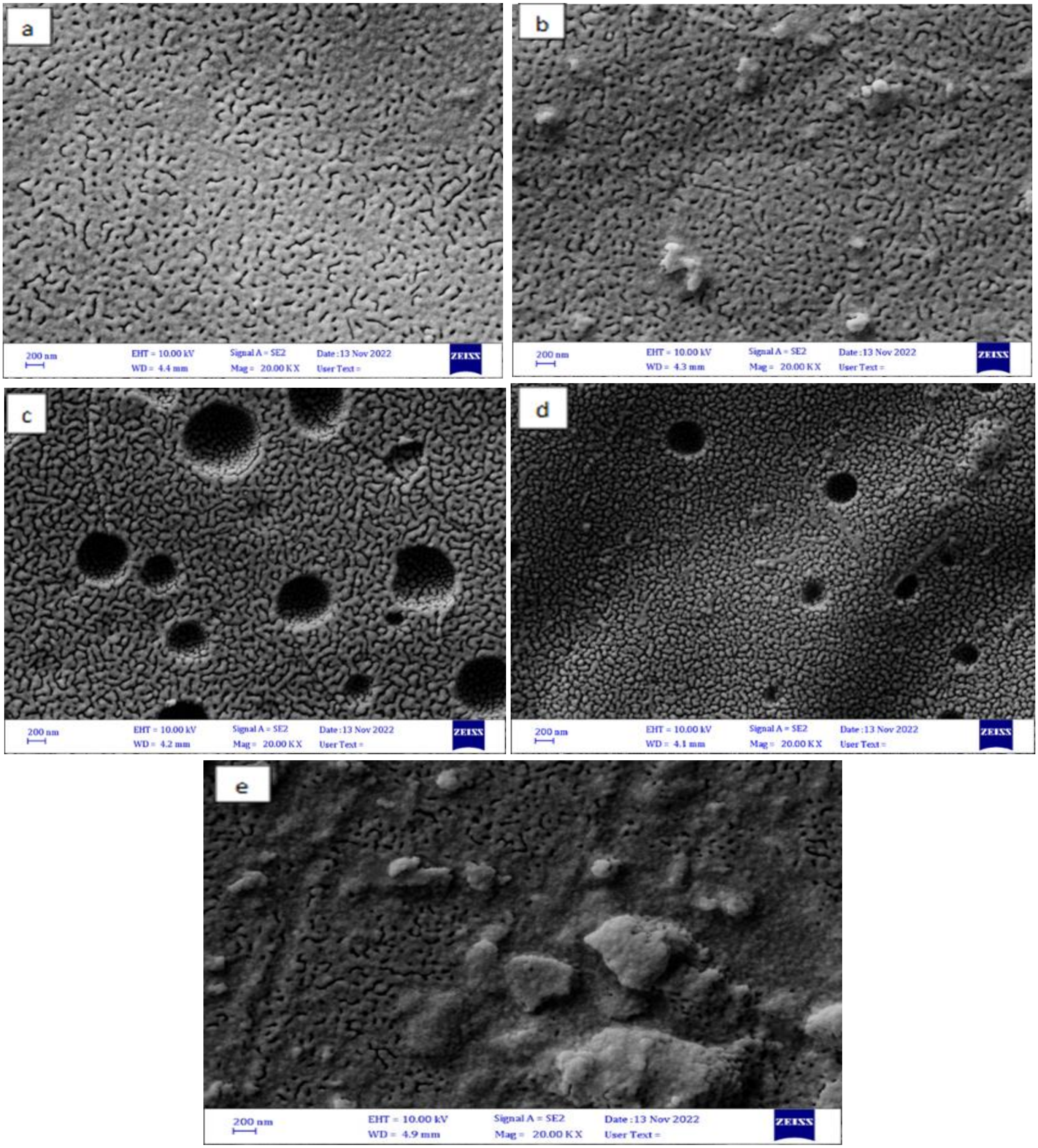
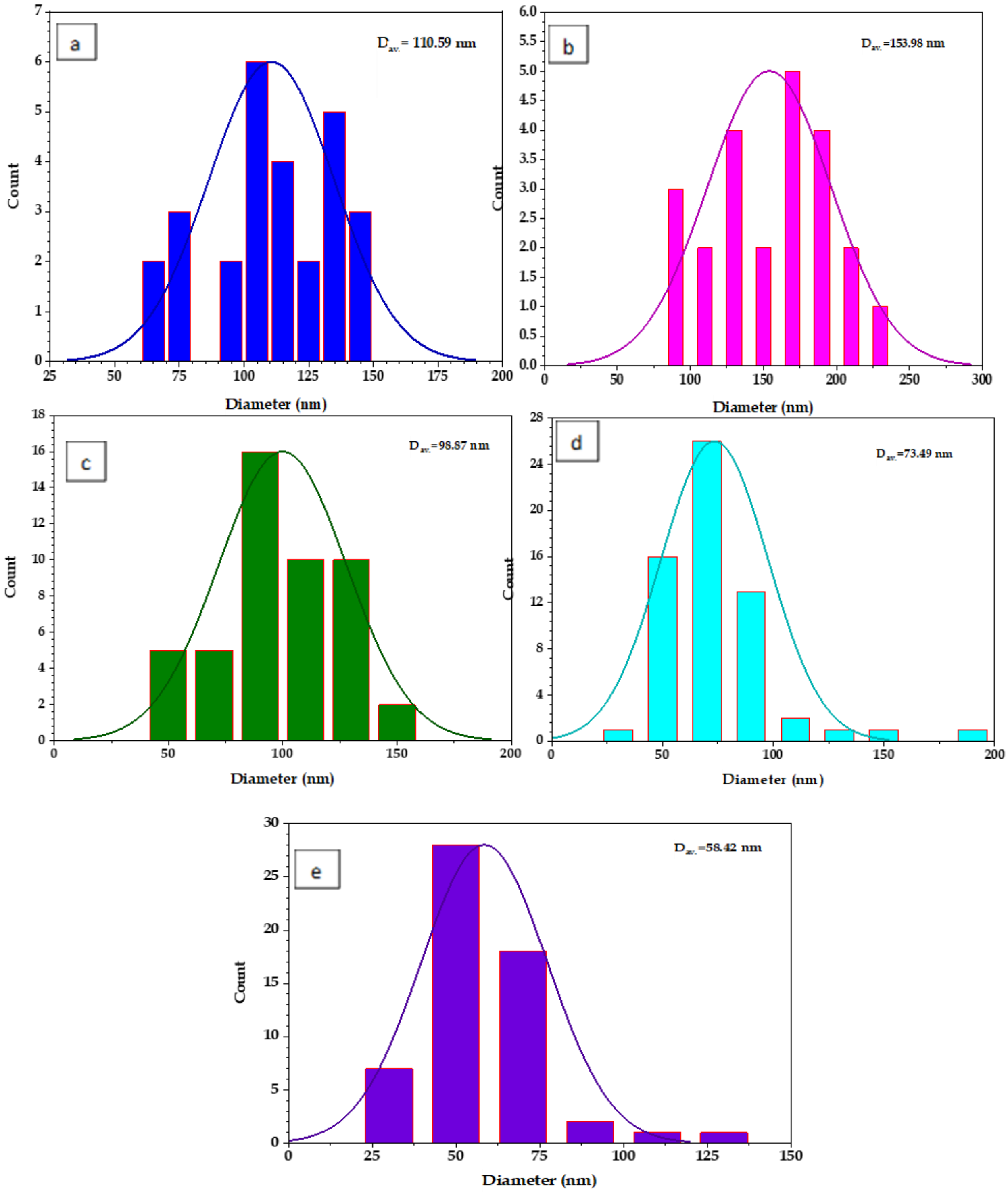


Figure (4.2) FE-SEM images (20KX)of PS/ SiC/Sb_2O_3 NC, (a) for (Ps), (b) 2 wt.% SiC/ Sb_2O_3 NPs, (c) 4 wt.% SiC/ Sb_2O_3, (d) 6 wt.% SiC/ Sb_2O_3NPs, (e) 8 wt.% SiC/ Sb_2O_3NPs



Figure(4.3)histogram of PS/ SiC/Sb_2O_3 NC, (a) for (Ps), (b) 2 wt.% SiC/ Sb_2O_3 NPs, (c) 4 wt.% SiC/ Sb_2O_3, (d) 6 wt.% SiC/ Sb_2O_3NPs, (e) 8 wt.% SiC/ Sb_2O_3NPs

4.2.3FourierTransform Infrared Radiation (FTIR) of (PS/SiC/Sb_2O_3) NCs

FTIR spectra of (PS/SiC/Sb_2O_3) nanocomposites in the range (100-4000) cm^{-1} are shown in figure (4.4). The absorption band of pure PS in the image A at 2980 cm^{-1} corresponding to the C-H stretching vibrations in the main chain and in aromatic rings[83]. The bands (1492.02 cm^{-1} and 1451.41 cm^{-1}) attributed to the C-H stretching vibrations [89]while the bands (748.55 cm^{-1} 694.93 cm^{-1} correspond to the C-H out phase bend [89]The spectra of polystyrene with additive different concentration of SiC and Sb_2O_3 NPs in images b, c, d and e respectively. In image B where the additive 2 wt.% from SiC and Sb_2O_3 NPs caused a shift to low wavenumber in some bands and intensities at (1451.37, 747.45, 694.43) cm^{-1} but bands 1492.02 cm^{-1} and 2980 cm^{1} there is not affected on this band. The image C which additive concentration of 4 wt.% from SiC and Sb_2O_3 NPs, the bands (1451.22, 747.37 cm^{-1}, 694.68) cm^{-1} was shifted to low wavenumber and the band 1492.02 cm^{-1} and 2980 cm^{1} there is not influenced. The bands (1451.27, 747.55 cm^{1}, 694.64) cm^{-1} in image D where additive 6wt.% from NPs, caused shift to low wavenumber while in the other hand, the band 1492.02 cm^{-1} and 2980 cm^{1} there is not change. From the additive concentration 8wt.% from NPs in image E, the band (1491.67, 694.64) cm^{-1} caused change to low wave number, while the band 748.03 cm^{-1} caused change to high wave number but the band 1451.37 cm^{-1} and 2980 cm^{-1} there is not affected. The FTIR proven that there is no chemical interactions between polystyrene and SiC and Sb_2O_3 NPs

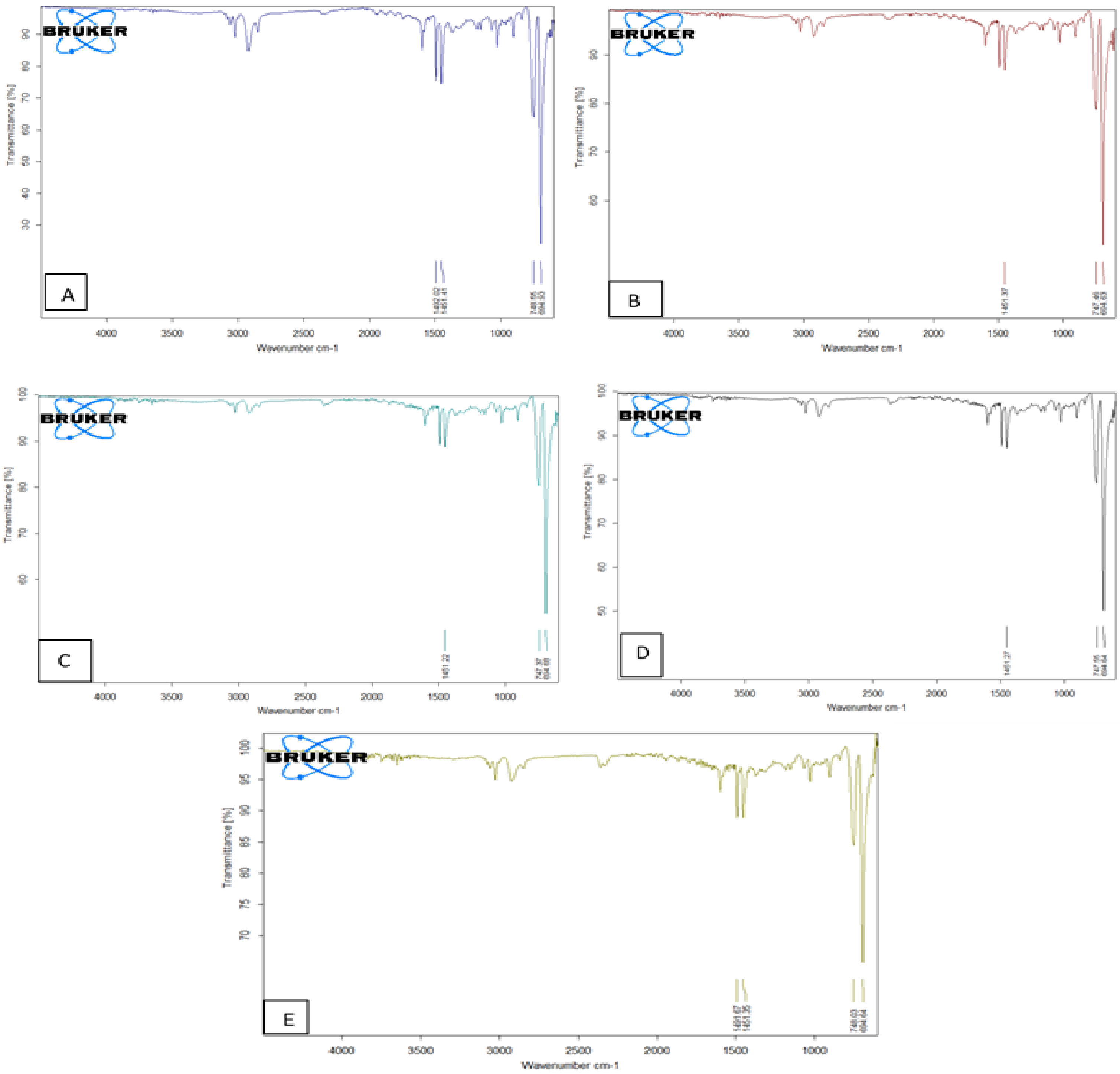


Figure (4.4) FTIR spectra for PS/ SiC/ Sb_2O_3 NPs: (A) for (Ps), (B) 2 wt.% SiC/Sb_2O_3 , (C) 4wt.% SiC/Sb_2O_3,(D) 6 wt.% SiC/Sb_2O_3, (E) 8 wt.% SiC/Sb_2O_3

4.3 The Optical Properties

The main purpose of studying the optical properties of the ($PS/SiC/Sb_2o_3$) nanocomposites is to identify the effect of adding the SiC/Sb_2O_3 nanoparticles on the optical properties of ($PS/SiC/Sb_2O_3$). The research involves measuring the absorbance spectrum of ($PS/SiC/Sb_2O_3$) films at room temperature, determining the absorption, extinction, and other optical constants, defining the forms of electronic transitions, measuring energy gaps.

4.3.1 Absorbance

Figure (4.5) shows the ($PS/SiC/Sb_2O_3$) nanocomposites' absorption spectra relative to the wavelength of the incident light. This graph shows how absorbance is highest for all films at wavelengths close to the critical absorption edge at (220 nm), and subsequently decreases when the wavelength is raised. Films typically absorb little in the visible and near infrared ranges. This behavior is demonstrated by the fact that, when incident photon wavelength decreases (near the fundamental absorption edge), the photon gains impartial sufficient energy to interact by atoms and go through matter. As wavelength decreases, photon contact with the material rises absorbance (near the fundamental absorption edge)[90]

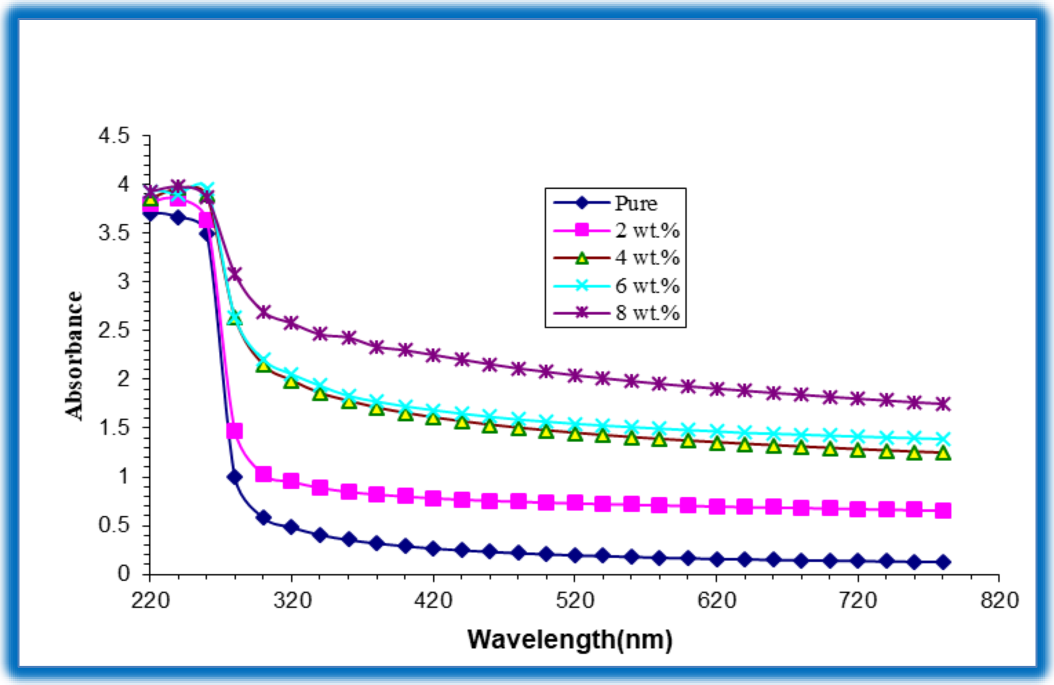
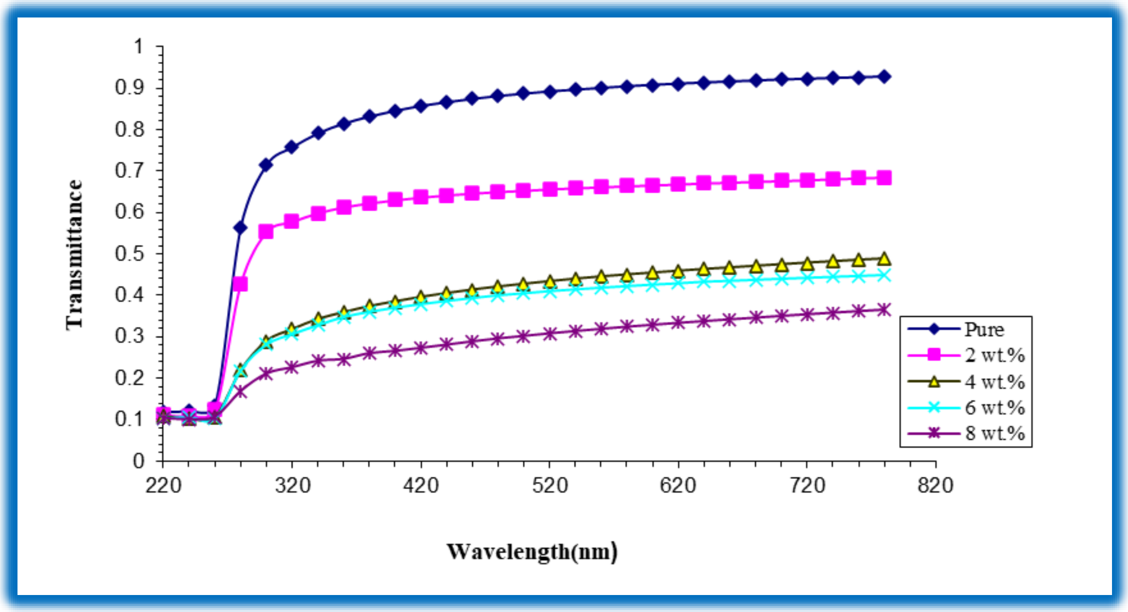


Figure (4.5) Difference of absorbance for (PS/SiC/Sb_2O_3) nanocomposites with wavelength

4.3.2 Transmittance Spectrum

Figure (4.6) illustrates how the optical transmittance spectrum for films made of (PS/SiC/Sb_2O_3) changes with wavelength when different ratios of SiC/Sb_2O_3 NPs are added. According to the graph, transmittance reduces when SiC/Sb_2O_3 NPs content rises. The additional SiC/Sb_2O_3 NPs include electrons in outer orbits that absorb the electromagnetic energy of the incident light and travel to the highest energy levels. Pure polystyrene, which has a high transmittance value but no free electrons, prevents radiation from being emitted in this situation since the electrons that have traveled to higher stages take occupied the open energy band locations. This causes some of the received light to be absorbed by the substance and not travel through it (electrons are linked to atoms by covalent bonds). For electrons to break free from their bonds and enter the conduction band, a high-energy photon is required[63, 91]



Figure(4.6) The transmittance for($PS/SiC/Sb_2O_3$)nanocomposites with wavelenth

4.3.3 Absorption Coefficient (α)

Equation (2.7) used to calculate the coefficient of absorption (cm^{-1}) figure (4.7) demonstrates how the ($PS/SiC/Sb_2O_3$) nanocomposites' absorption coefficient varies with photon energy. The absorption coefficients are lowest at high wavelengths and low energies, as can be seen by looking at them. This implies that there is minimal likelihood of an electron being displaced as a result of low energy photons ($h\nu > E_g^{op)}$ [92] because of the strong absorption at high energies, there is a higher likelihood that electrons may migrate around. The photon that entered has sufficient energy to make the transition from the valence bands to the conduction bands, therefore the gap of energy is smaller than the energy of the incident photon. This shows how the coefficient of absorption influences the type of electron transition; at high energies, the coefficient of absorption is predicted to be great ($>10^4$ cm^{-1}), revealing that direct electron transitions occur, with electrons and photons maintaining the energy and moment; at low energies, the coefficient of absorption (10^4) cm^{-1}, denoting that indirect transitions occur, and the electric momentum is reinforced by the phonons[93]The (PS/SiC/Sb_2O_3) nanocomposites' coefficient of absorption is below (10^4 cm^{-1}), among other findings, suggesting an indirect electron transition

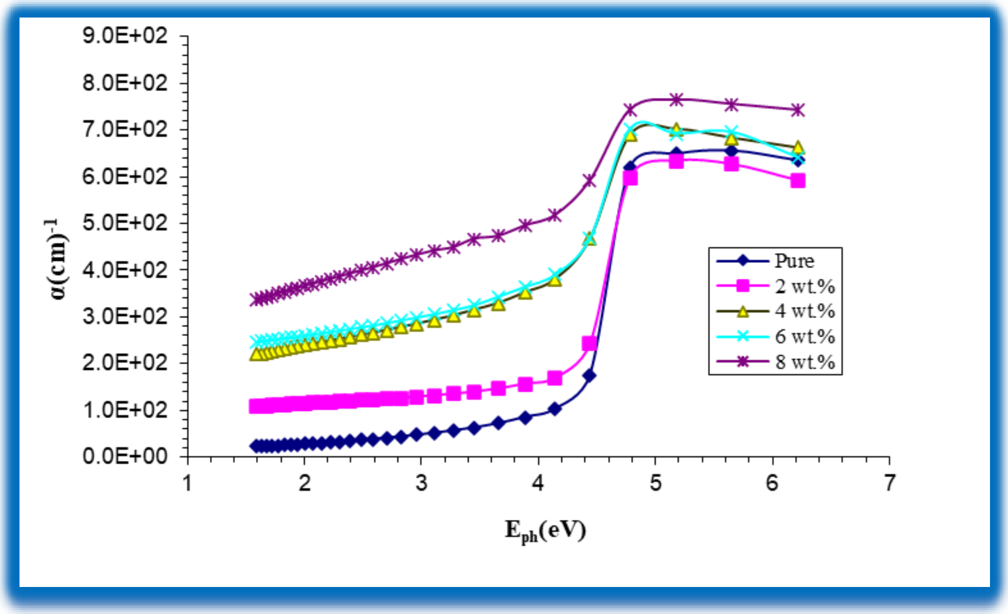


Figure. (4.7) the coefficient of absorption of (PS/SiC/Sb_2O_3) nanocomposites with energy of photon

4.3.4 The (Allowed and Forbidden) Indirect Transition's Optical Energy Gap

Equation (2.3) has been used to calculate the permitted and forbidden indirect transition band energy gaps for (PS/SiC/Sb_2O_3) nanocomposites. The values of the gap of energy for permitted and banned indirect transitions, individually, are shown in figures (4.8) and (4.9). With increasing silicon carbide (SiC) and antimony trioxide (Sb_2O_3) nanoparticles concentration, the energy gap values for permitted and banned indirect transitions are decreases. This drop is due to the fact that silicon carbide (SiC) and antimony trioxide (Sb_2O_3) nanoparticles content causes some film defects to occur. Local states in the optical band gap and overlap are created by these imperfections. These overlaps provide evidence that the energy band gap decreases as the proportion of silicon carbide (SiC) and antimony trioxide (Sb_2O_3) nanoparticles in the polymeric matrix rises. On the other hand, the rise in the level of disorder in the films is a direct result of the smaller optical gap[94] The values of the energy gap of nanocomposites are listed in Table (4.1)

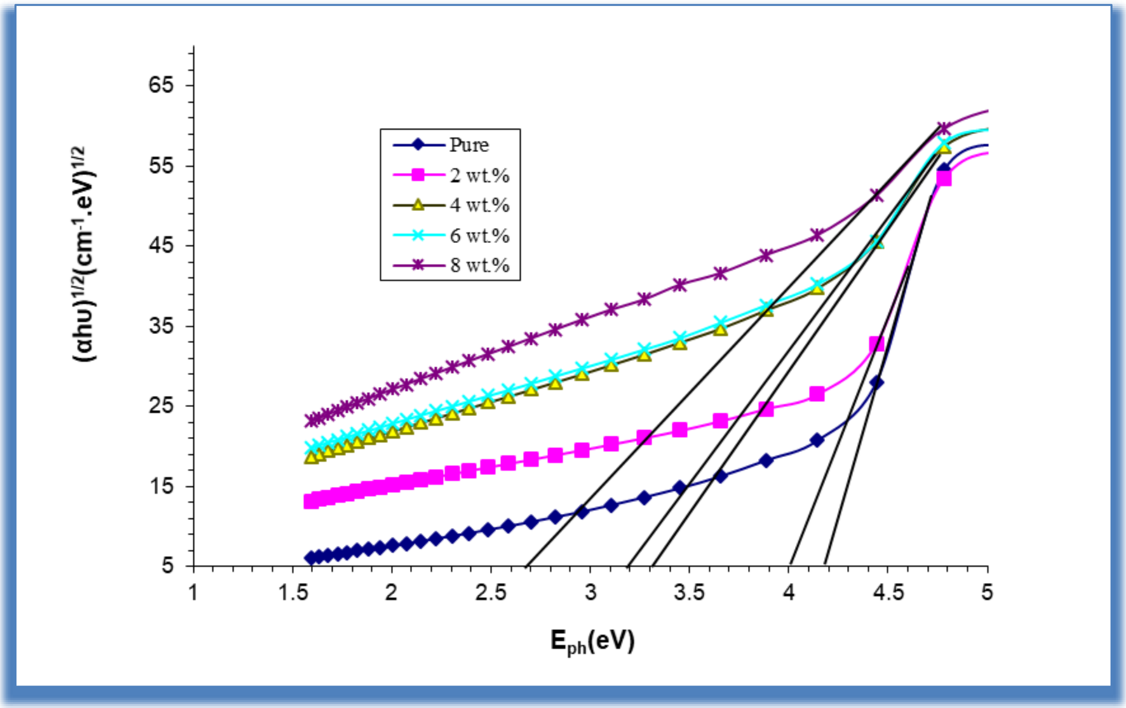


Figure (4.8) The relationship between $(\alpha h\upsilon)^{1/2}(cm^{-1}.eV)^{1/2}$ and photon energy of $(PS/SiC/Sb_2O_3)$ nanocomposites

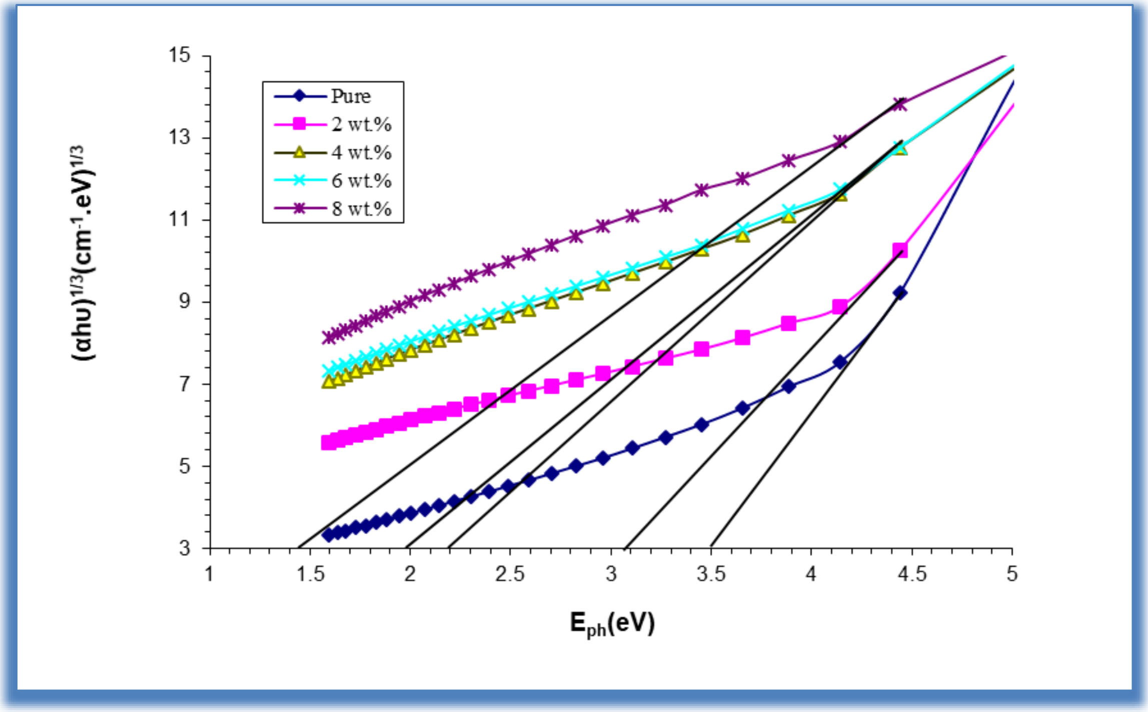


Figure (4.9) The relationship between $(\alpha h\upsilon)^{1/3}(cm^{-1}.eV)^{1/3}$and photon energy of ($PS/SiC/Sb_2O_3$) nanocomposites.

Table (4.1) Values of energy gap of ($PS/SiC/Sb_2O_3$) nanocomposites

SiC/Sb_2O_3NPs wt% content	Allowed of indirect energy gap (eV)	Forbidden of indirect energy gap (eV)
0	4.19	3.5
2	4	3.2
4	3.3	2.2
6	3.1	1.9
8	2.69	1.45

4.3.5 Refractive Index

Equation (2.12) is used to compute the refractive index (n). Figure (4.10) shows the ($PS/SiC/Sb_2O_3$) nanocomposites' refractive index as a function of wavelength. The figure shows that the index of refractive varies with rising weight percentages of SiC/Sb_2O_3 nanoparticles added to polystyrene due to the increased density of nanocomposites (PS). Owing to the area's small transmittance, the UV region has in height index of refractive values, whereas the visible zone has small values as a result of the region's high transmittance[95]

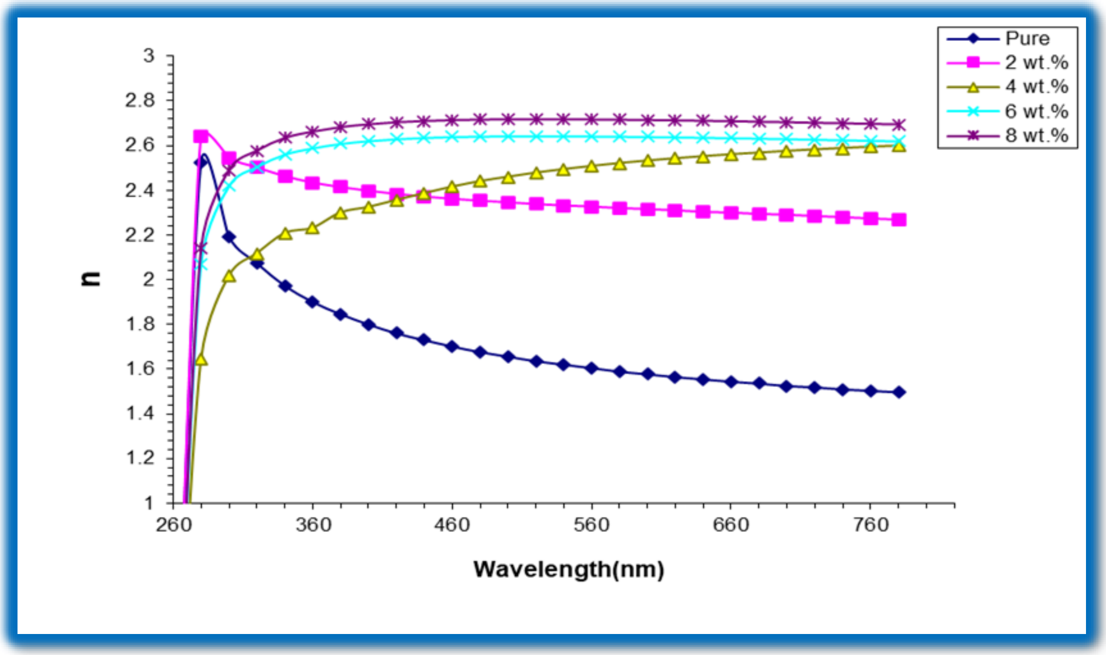


Figure (4.10) the refractive index of ($PS/SiC/Sb_2O_3$) nanocomposites as a function of wavelength.

4.3.6 Extinction Coefficient

The coefficient of extinction (k) is obtained by the eqation (2.8). Figure (4.11) demonstrate the coefficient of extinction for (PS/SiC/Sb_2O_3) nanocomposites with wavelength. The coefficient of extinction is smaller at low concentrations and rises as SiC/Sb_2O_3 NPs content raised. This is due to the fact that the coefficient of absorption rise with the content of SiC/Sb_2O_3 NPs rises, this discovery indicates that the atoms of the SiC/Sb_2O_3 nanoparticles will affect the structure of the host polymer[96]

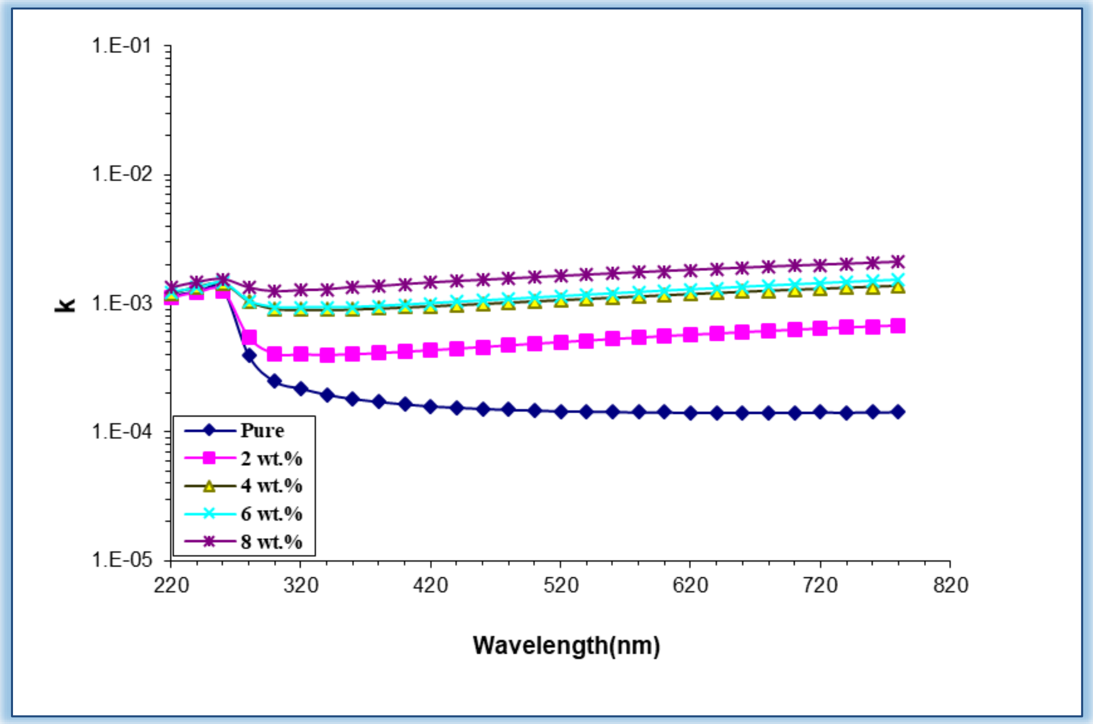


Figure (4.11) Variation of extinction coefficient of (PS/SiC/Sb_2O_3) nanocomposites with wavelength

4.3.7 Real and Imaginary Parts of Dielectric Constant

Figures (4.12) and (4.13) illustrate the real dielectric constant and imaginary dielectric constant of (PS/SiC/Sb_2O_3) nanocomposites as functions of wavelength, respectively, which is the ratio between the imaginary and real portions of the dielectric constant, is known from the data of the real and imaginary parts of the dielectric constant. It can be claimed that the part of real is larger than the part of imaginary since the real component is primarily proportionate to the square of the refractive index (n). The imaginary component varies with the extinction coefficient (k) in a direct proportion[97]

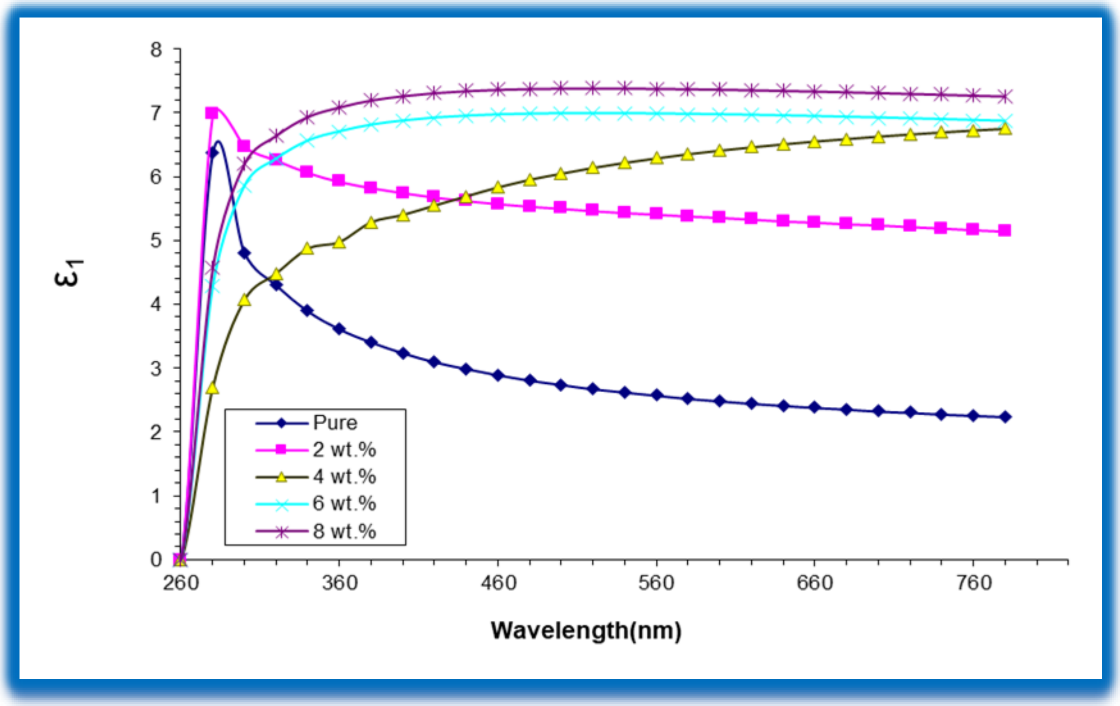


Figure (4.12) the real dielectric constant as a function of incident wavelength for (PS/SiC/Sb_2O_3) Nanocomposites

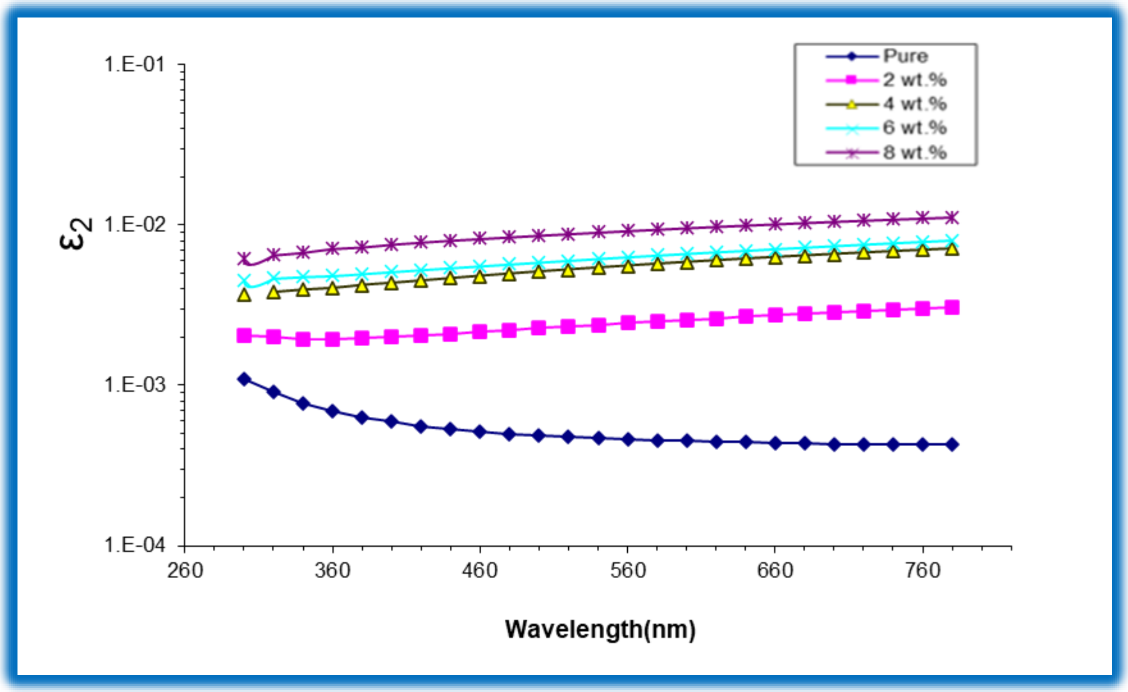


Figure (4.13) the imaginary dielectric constant as a function of wavelength for (PS/SiC/Sb_2O_3) nanocomposites

4.3.8 Optical Conductivity

Equation (2.18) is utilized to determine optical conductivity. The relationship between optical conductivity and wavelength is seen in figure (4.14). The conductivity of optical reduces with rising SiC/Sb_2O_3 NPs content, according to observations; additionally, the inclusion of SiC/Sb_2O_3 NPs improves the optical conductivity of (PS/SiC/Sb_2O_3) nanocomposites. This phenomenon is brought on by the absorption coefficient[98]

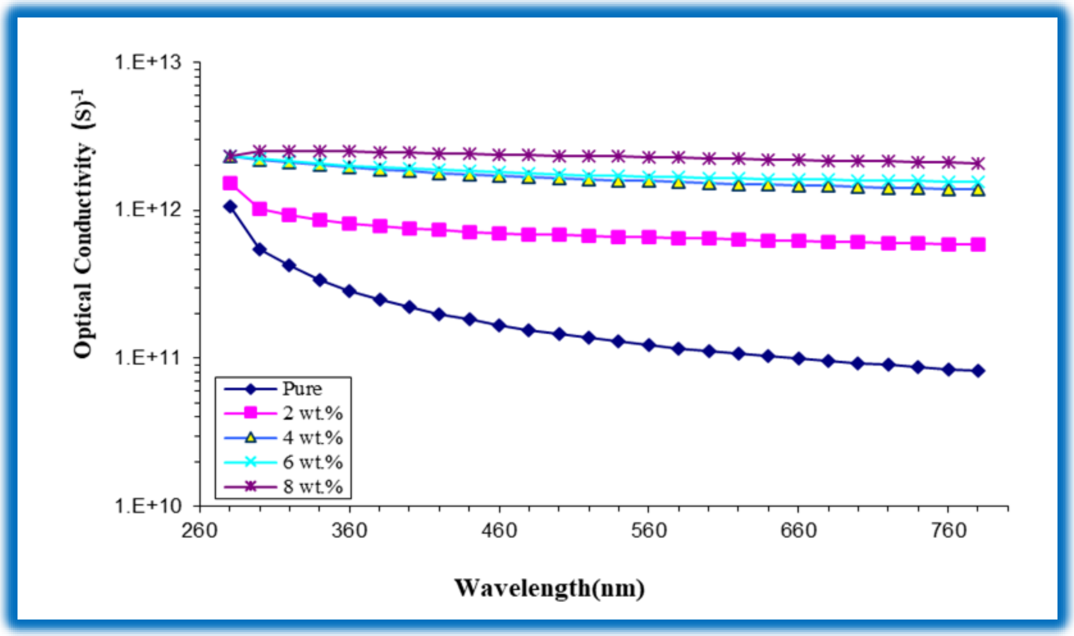


Figure (4.14) Optical conductivity of (PS/SiC/Sb_2O_3) nanocomposites as a function of wavelength

4.4 A.C Electrical Properties of (PS/SiC/Sb_2O_3) Nanocomposites

4.4.1 The Dielectric Constant of (PS/SiC/Sb_2O_3) Nanocomposites

Equation (2.22) was used to calculate the dielectric constant of (Ps/SiC/Sb_2O_3) nanocomposites. The variation of the dielectric constant with frequency is shown in Figure. (4.15) As can be observed, the dielectric constant values drop with increasing applied frequency, which leads to a reduction in the space charge to total polarization ratio. At low frequencies, space charge polarization is the most significant type of polarization, and as frequency rises, its significance decreases. As the electric field frequency rises, different kinds of polarizations take place, and the dielectric constant values for all samples of (Ps/SiC/Sb_2O_3) drop. Ionic polarization responds to variations in field frequency in a slightly different manner than electronic polarization because an ion has a larger mass than an electron[99,100]

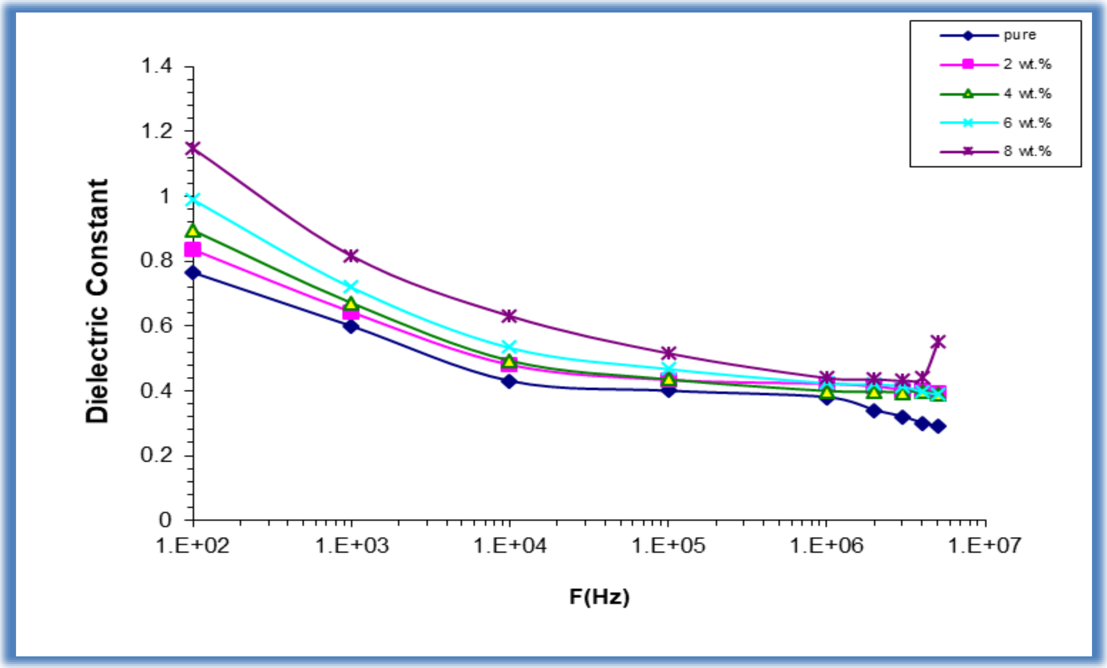


Figure (4.15) dielectric constant of ($PS/SiC/Sb_2O_3$) varies with frequency

The dielectric constant variation for ($PS/SiC/Sb_2O_3$) NCs at 100Hz is shown in figure. (4.16) relation to nanoparticle concentrations. As the percentage of SiC and Sb_2O_3 NPs rise, the dielectric constant of nanocomposites also rises. Interfacial polarization, a process that occurs when two surfaces within NCs are separated by an alternating electric field and causes a rise in charge carriers, could be used to explain this activity[95,101]

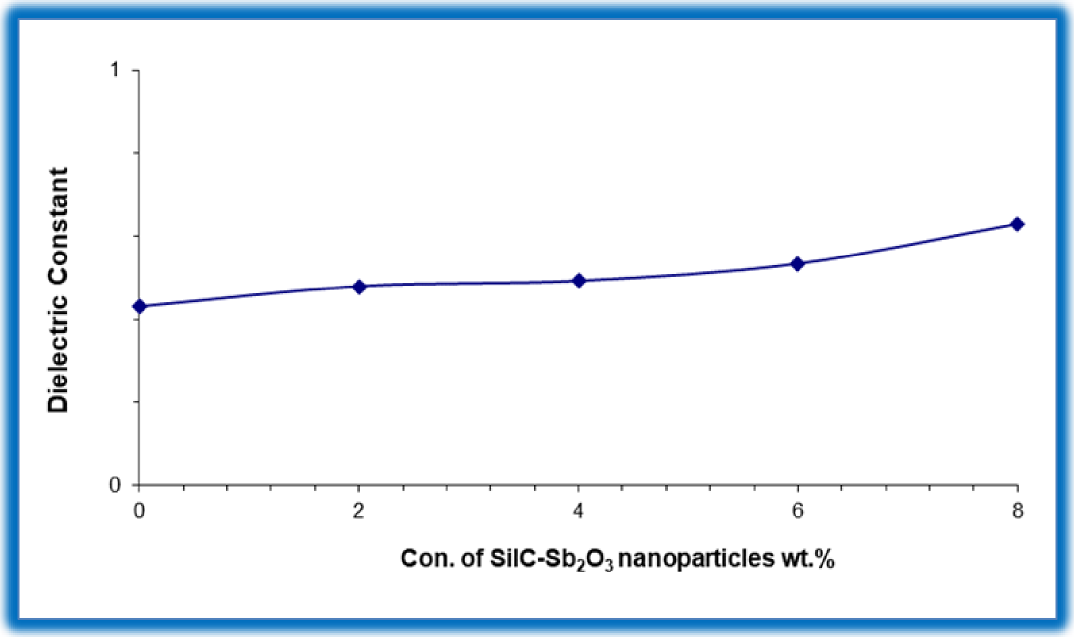


Figure (4.16) Difference of dielectric constant with concentration of (PS/SiC/Sb_2O_3) nanocomposite.

4.4.2 The Dielectric Loss of (PS/SiC/Sb_2O_3) Nanocomposite

Equation (2.23) was used to calculate the dielectric loss of the nanocomposites. Figure (4.17) show the dielectric loss of (Ps/SiC/Sb_2O_3) nanocomposites with the relation of frequency. From this figure it can be see the dielectric loss is high at lower applied frequencies, but decreases with increasing applied frequencies. This can be attributed to the actuality that as the frequency rises, the space charge polarization contribution decreases [102]

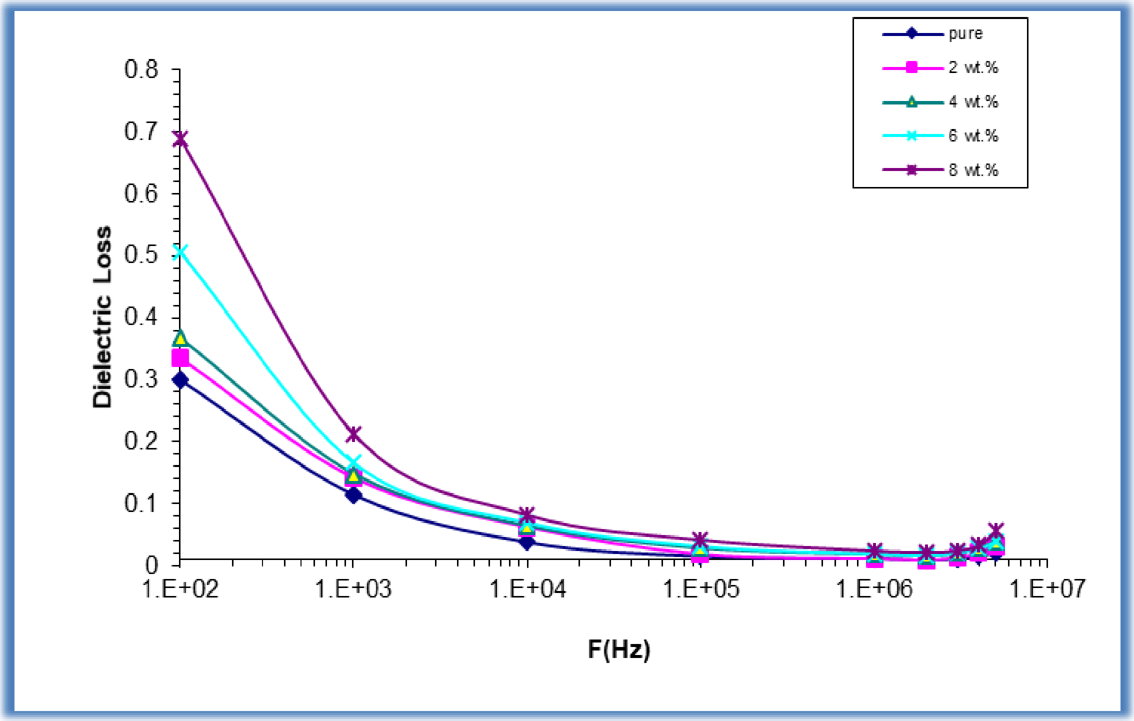


Figure (4.17) Dielectric loss variation with frequency for (PS/SiC/Sb_2O_3) nanocomposites

The relationship between SiC / Sb_2O_3 NPs concentration and dielectric loss is shown in Figure (4.18) as the concentration of NPs rises, the dielectric loss of (Ps/SiC/Sb_2O_3) NCs also rises, which is related to an increase in charge carriers[101]

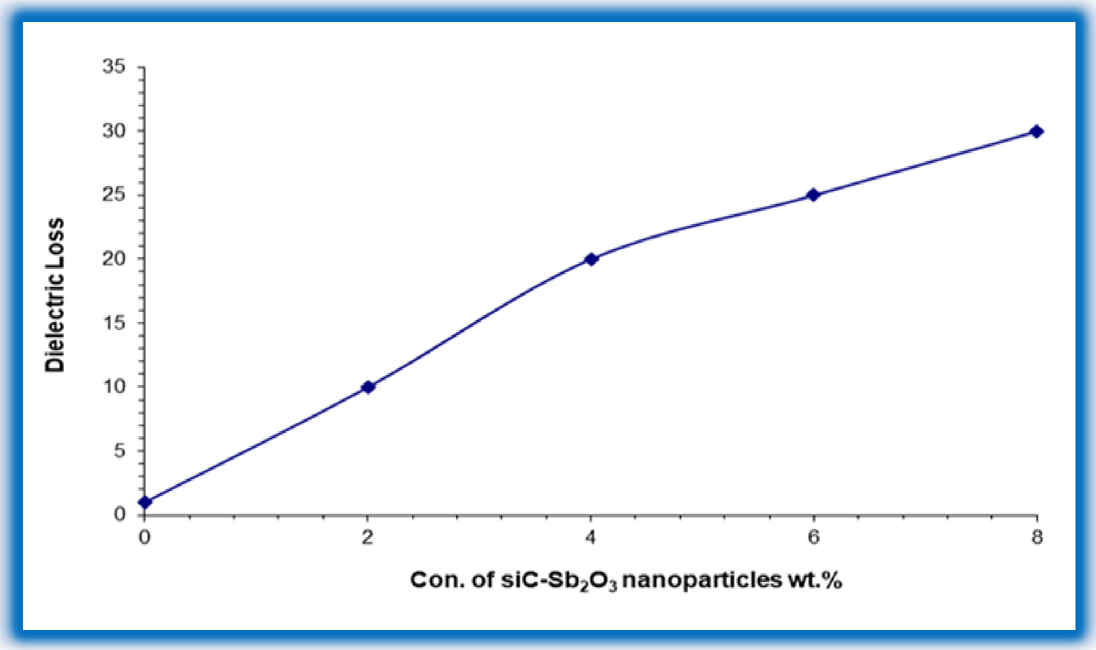


Figure (4.18) Difference of dielectric loss for (PS/ SiC/Sb_2O_3) NCs with different concentrations of (Sic/Sb_2O_3) NPs

4.4.3 A.C Electrical Conductivity of (PS/SiC/Sb_2O_3) Nanocomposites

The A.C Electrical conductivity was calculated from equation (2.24) figure (4.19) showed the variation in conductivity of (PS/SiC/Sb_2O_3) NCs with frequency. This figure demonstrates that electrical conductivity significantly rises with frequency, which is caused by space charge polarization, which happens at low frequencies, and the hopping process, which causes charge carriers to move. The increase in electrical conductivity is only moderate at high frequencies due to electronic polarization and charge carriers that move through hopping[102]

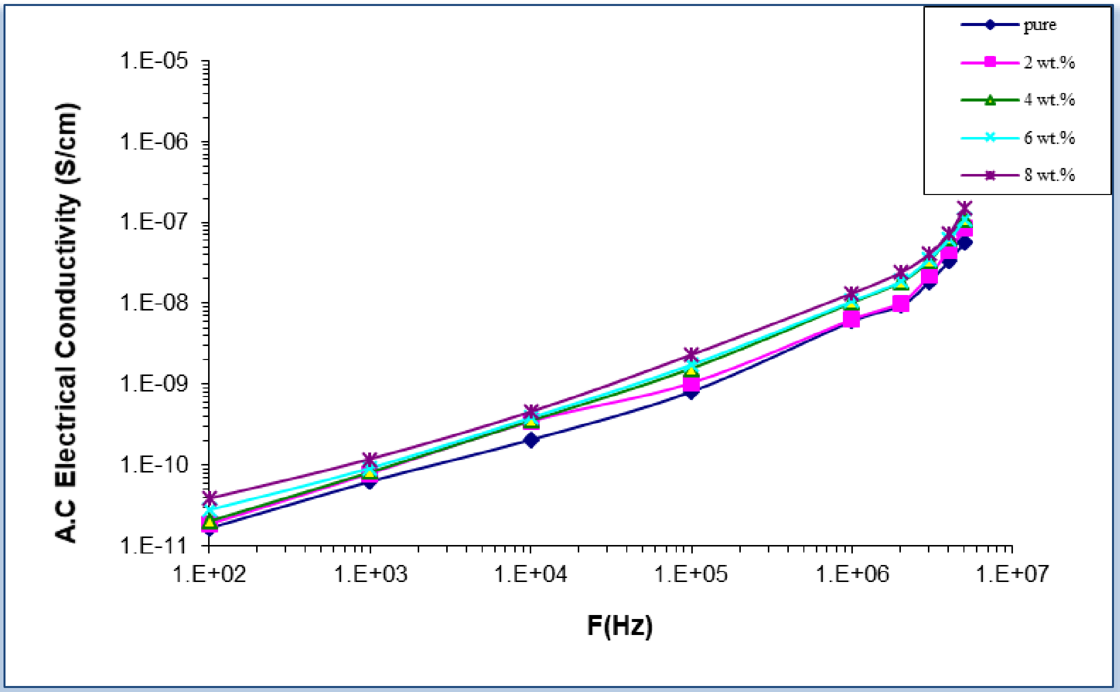


Figure (4.19) Difference of A.C electrical conductivity with frequency for (PS/SiC/Sb_2O_3) NCs

Figure. (4.20) the influence of SiC / Sb_2O_3 NPs on the A.C electrical conductivity of (PS/SiC/Sb_2O_3) NCs at 100 Hz. The A.C. electrical conductivity of NCs rises as SiC and Sb_2O_3 NPs concentration rises. Due to the composition of the dopant nanoparticles, there are more charge carriers, which reduces the NCs resistance and boosts electrical conductivity [100].Table(4.2) shows the relationship between concentrations and dielectric constant, dielectric loss and A.C electrical conductivity

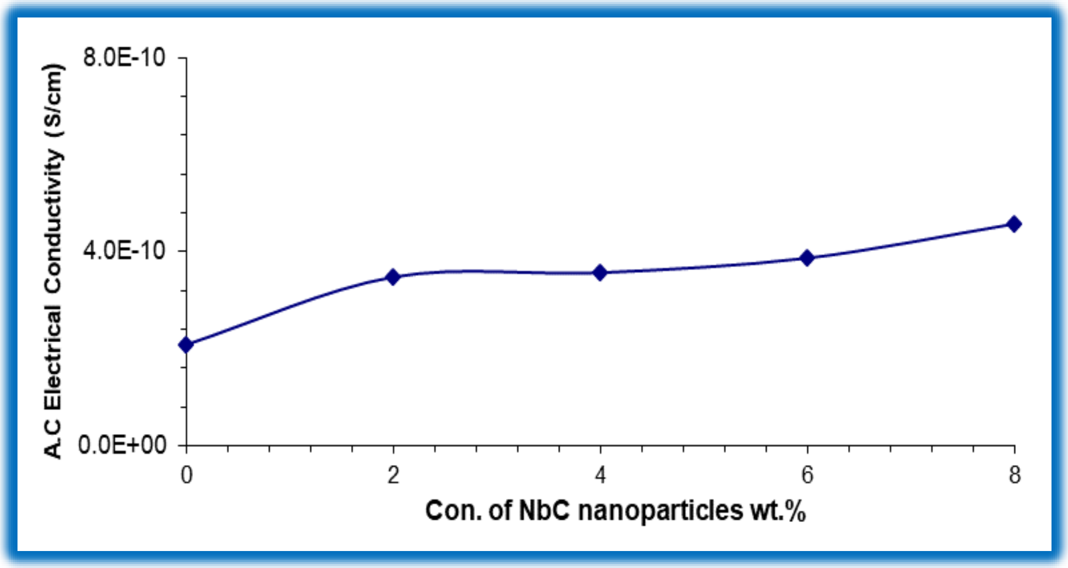


Figure (4.20) Difference of A.C electrical conductivity with (Sic/Sb_2O_3) NPs for ($Ps/SiC/Sb_2O_3$) NCs

Table (4.2) showing the relationship between concentrations and dielectric constant, dielectric loss and A.C electrical conductivity

Con(wt.)%	Dielectric constant	Dielectric loss	A.c electric conductivity
0	0.43	1	2.08E-10
2	0.479	10	3.47E-10
4	0.492	20	3.56E-10
6	0.534	25	3.86E-10
8	0.63	30	4.56E-10

4.5 Applications of (PS/SiC/Sb_2O_3) Nanocomposites For Antibacterial Activity

The antibacterial activity of the PS/SiC/Sb_2O_3 NCs samples was established against gram positive (*Staphylococcus*) and gram negative (*klebsiella*) bacteria. As seen in figures (4.21), (4.22), and (4.23) the inhibition zone widens as SiC/Sb_2O_3 NP concentrations rise. The antibacterial activity of PS/SiC/Sb_2O_3 NCs might be due to responsive oxygen species (ROS) produced by various NPs concentrations. The antibacterial activity of NCs may be owing to a chemical reaction between membrane proteins and hydrogen peroxide; this reaction results in the production of hydrogen peroxide, which enters bacterial cell membranes and kills the bacteria. Another potential mechanism of action is that the positive charges on the nanoparticles in NCs and the negative charges on the microorganisms cause an electromagnetic attraction among them. The germs oxidize and perish when the attraction forms[103,104] The findings demonstrated that adding SiC/Sb_2O_3 NPs improved the antibacterial activity of the films made of PS/ SiC/Sb_2O_3NCs. Chemistry, particle size, particle shape, and zeta potential are some of the factors influencing antibacterial activity that are most significant[105]

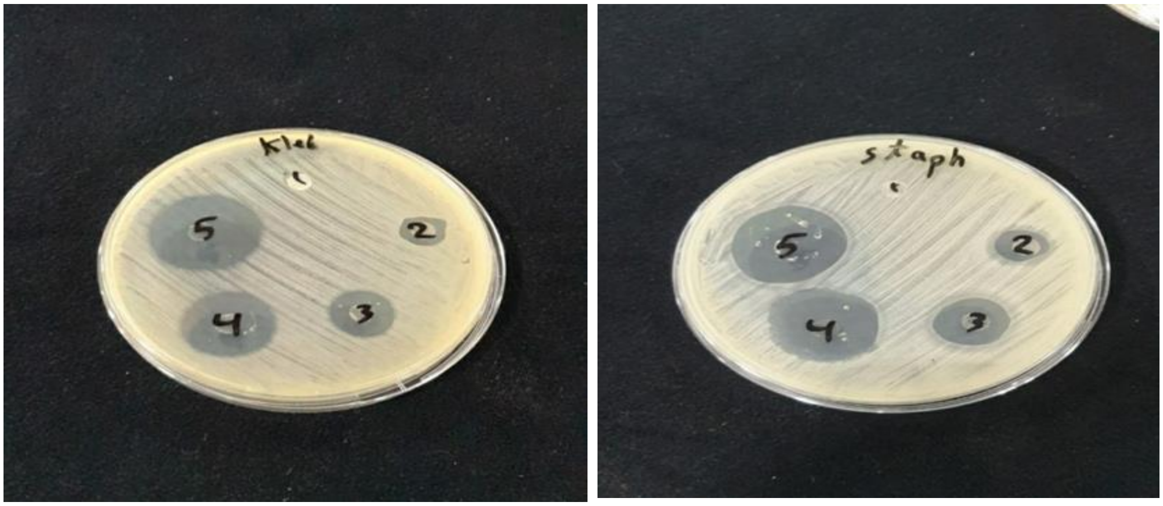


Figure (4.21) Images for inhibition zones of (PS/SiC/Sb_2O_3) nanocomposite films on S. aureus and K. aerogenes

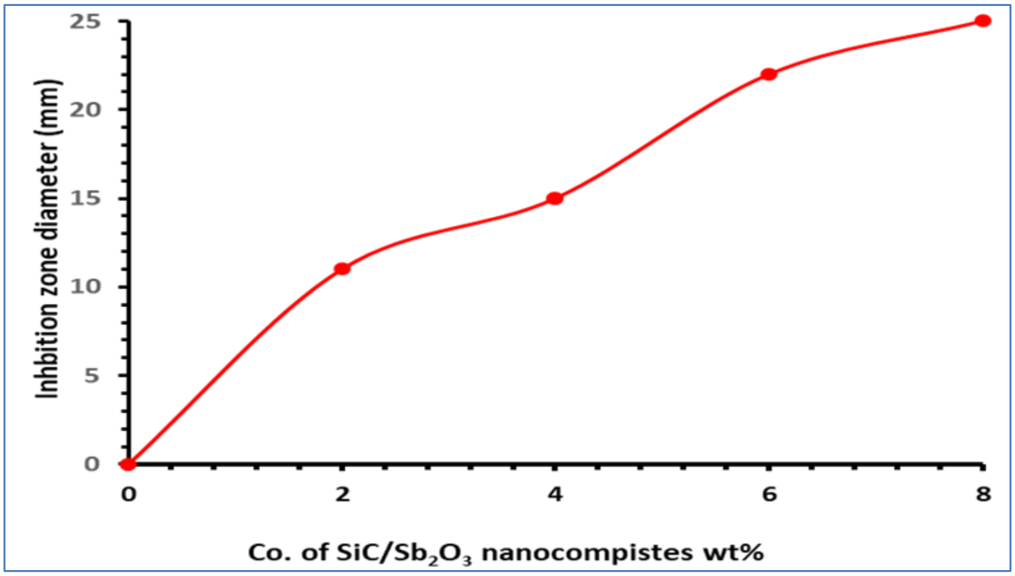


Figure (4.22) Antibacterial effect of polystyrene as a function of SiC/Sb_2O_3nanopartical concentrations on (Staphylococcus).

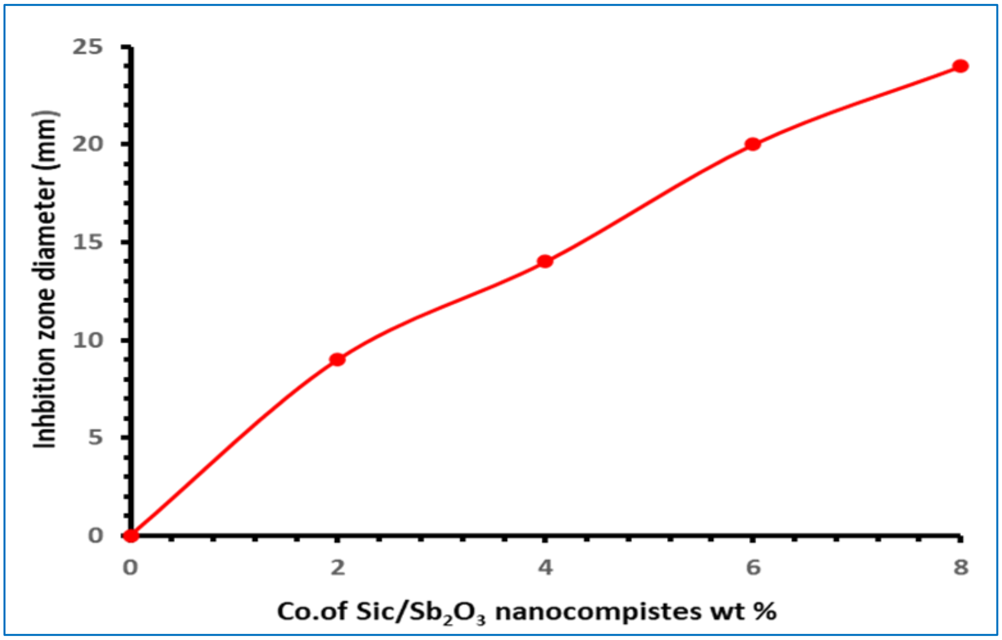


Figure (4.23) Antibacterial effect of polystyrene as a function of SiC/Sb_2O_3nanopartical concentrations on (Klebsilla).

4.6 Conclusion

1- The photos taken with an optical microscope (OM) show that when silicon carbide (SiC) and antimony trioxide (Sb_2O_3) nanoparticles are present in a (8) wt.% concentration, they form a continuous network within the polymer.

2-The surface morphology of the (PS/SiC/ Sb_2O_3) nanocomposites films is shown by (FE-SEM) images, which are composed of numerous chunks randomly or aggregates scattered throughout the upper surface but are coherent and homogeneous.

3-The Fourier transformation spectroscopy (FTIR) confirmed the additive SiC/ Sb_2O_3 NPs caused interaction with polymer matrix. The FTIR proven that there is physical interactions between polystyrene polymer matrix and SiC / Sb_2O_3 NPs.

4-The optical characteristics experimentations exposed that the absorbance, index of refractive, coefficient of extinction, coefficient of absorption, dielectric constant (imaginary and real), and conductivity of optical of (PS/SiC/ Sb_2O_3) nanocomposites increase as the SiC/Sb_2O_3 nanoparticles increase, while the transmittance decreases. For allowed and forbidden indirect transitions, the gap of energy reduces from (4.19 eV to 2.69 eV) and (3.5 eV to 1.45 eV), respectively. The optical properties of the (Ps/SiC/ Sb_2O_3) nanocomposites suggested that they could be used in a variety of electronic and photonic applications.

5- The dielectric constant and dielectric loss of (Ps/SiC/Sb_2O_3) decreased with increasing frequency and increased with increasing concentration of (SiC/Sb_2O_3) nanoparticles. The A.C electrical conductivity of (Ps/SiC/Sb_2O_3) increased with increasing frequency and concentration of (SiC/Sb_2O_3) nanoparticles.

6- The inhibition zone values of Klebsiella and Staphylococcus bacteria increased by increasing the SiC/Sb_2O_3 NPs ratio in polystyrene to 24 and 25 mm respectively. These PS/SiC/Sb_2O_3 nanocomposite spheres have outstanding antibacterial properties against Staphylococcus and Klebsiella, according to preliminary antibacterial testing. These PS/SiC/Sb_2O_3 nanocomposite spheres, in our opinion, can be widely used as recyclable catalysts for reducing organic dyes in wastewater treatment as well as an antibacterial agent for use in medical and environmental applications.

4.7 Future Work

1- Studying the thermal and mechanical properties of (PS/SiC/Sb_2O_3) NCs

2-Studying the rheological properties of (PS/SiC/Sb_2O_3) NCs

3-Studying the D.C electrical properties of (PS/SiC/Sb

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