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Influence of BaTiO₃ and TiO₂ Nanoparticles on Biopolymer Properties for Environmental Applications

A thesis

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By

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بِسْمِ اللَّهِ الرَّحْمَنِ الرَّحِيمِ

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المجادلة {11}

Dedications

To mesopotamia(Iraq) with honour and dignity...

*the one who laid the rules for generous creation, and how to restrain the
reins of the soul ... my father's spirit.*

To my mother whose love is planted in my heart...

To my brothers and sisters...

To my close friends

To my teachers

Who provide me the keys of success

Zainab

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Summary

The (PVA-BaTiO₃-TiO₂) nanocomposites have been prepared by solution cast method with different concentrations (0,1,1.5,2 and 2.5) wt.% of barium titanate and titanium dioxide nanoparticles . The structural, optical and (A.C) electrical properties of nanocomposites have been studied. The structural properties include: Fourier Transform Infrared Ray (FTIR), Scanning Electron Microscope (SEM) and optical microscope (OM). The results of optical microscope and SEM image showed good distribution of barium titanate and titanium dioxide nanoparticles inside PVA . The results of (FTIR) showed that all peaks of the most bond remain in the same wave number. The results of optical properties for (PVA-BaTiO₃-TiO₂) nanocomposites showed that the absorbance, absorption coefficient, extinction coefficient, refractive index, real and imaginary dielectric constants, optical conductivity was increased with the increase of BaTiO₃ and TiO₂ nanoparticles concentrations while the transmittance and energy band gap were decreased with the increase of BaTiO₃ and TiO₂ nanoparticles concentrations. Nanocomposites have a high absorption for UV region. The results of the A.C electrical properties of nanocomposites revealed that the dielectric constant and dielectric loss of nanocomposites were decreased as the frequency of applied electric field increased, and increased as the concentrations of BaTiO₃ and TiO₂ nanoparticles increased, while the A.C electrical conductivity was increased with increasing of the frequency and with increasing the BaTiO₃ and TiO₂ nanoparticles concentrations. The results of antibacterial applications of (PVA-BaTiO₃-TiO₂) nanocomposites showed that the inhibition zone for gram-positive and gram-negative was increased with increase the concentrations of BaTiO₃ and TiO₂ nanoparticles.

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List of Symbols

<i>Symbols</i>	<i>Physical Meaning</i>
n	<i>Refractive Index</i>
k₀	<i>Extinction Coefficient</i>
A	<i>Absorbance</i>
I₀	<i>Incident Intensity of Light</i>
T_r	<i>Transmittance</i>
α	<i>Absorption coefficient</i>
h	<i>Plank constant</i>
λ	<i>Wavelength of light</i>
N	<i>Complex refractive index</i>
D	<i>Dispersion Factor</i>
ε₁	<i>Real dielectric constant</i>
ε₂	<i>Imaginary dielectric constant</i>
ε'	<i>Dielectric constant</i>
E	<i>Energy</i>
n	<i>Load carrier</i>
R	<i>Reflectance</i>
t	<i>Thickness</i>
ε	<i>Complex dielectric constant</i>
σ_{op}	<i>Optical Conductivity</i>

K_B	<i>Boltzmann constant</i>
P	<i>Polarization</i>
N_o	<i>Number of molecules per a unit of volume</i>
μ_i	<i>Electrical dipole moment</i>
ϵ_o	<i>Vacuum permittivity</i>
V_m	<i>Maximum voltage</i>
i	<i>Imaginary number</i>
ω	<i>Angular frequency</i>
C	<i>Capacitance</i>
I	<i>Electrical current</i>
R_p	<i>Parallel resistance</i>
B	<i>Constant depended on type of material</i>
μ	<i>linear attenuation coefficients</i>

List of Abbreviations

Symbol	Physical meaning
PVA	<i>Polyvinyl Alcohol</i>
BaTiO₃	<i>Barium Titanate</i>
TiO₂	<i>Titanium Dioxide</i>
FTIR	<i>Fourier Transformation Infrared Ray</i>
SEM	<i>Scanning Electron Microscope</i>
Vis	<i>Visible</i>
UV	<i>Ultra Violet</i>

IR	<i>Infrared</i>
C.B	<i>Conduction Band</i>
V.B	<i>Valence Band</i>
A.C	<i>Alternating current</i>
PEG	<i>Polyethylene glycol</i>
PEO	<i>Polyethylene Oxides</i>

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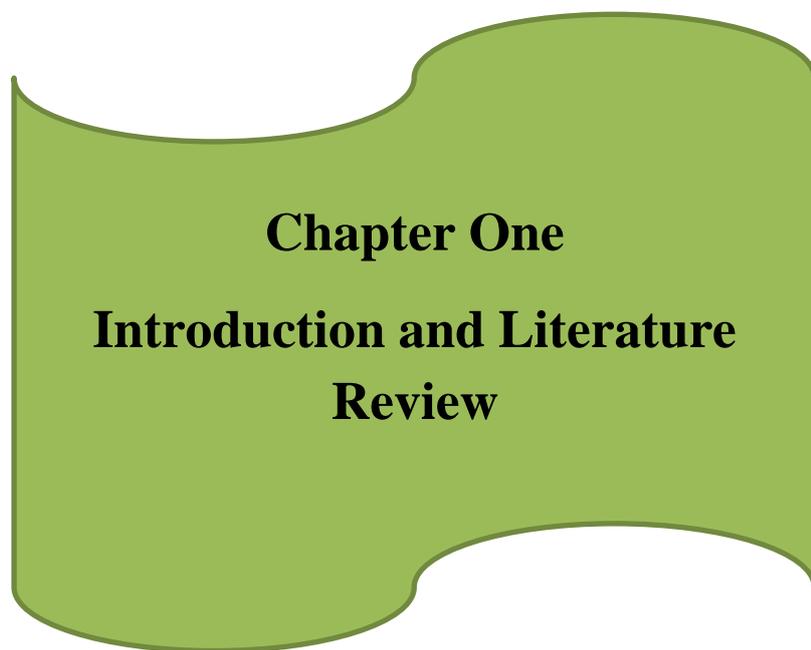
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Chapter One

Introduction and Literature Review

1.1 Introduction

Nanotechnology is a rapidly emerging interdisciplinary technology that has exploded in popularity in a number of fields in over the last ten years in the fields of the materials sciences, mechanics, electronics, optics, medicine, oil and airspace. The prefix "nano" was derived from the Greek word which means "dwarf ". The word "nano" means very small. one nanometer (nm) is one billionth of a meter, and it is equivalent to ten angstroms. As such, a nanometer is 10^{-9} meter, and it is 10000 times smaller than the diameter of a human hair. A human hair diameter is about 50 microns in size [1]. 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 nuclear matter with extreme precision [2]. Nanotechnology applications have only expanded in recent years, with the field of materials having the most potential, followed by electronics and medicine the following are some examples of nanotechnology's possible applications photovoltaic solar miniature thin film cells for efficient energy generation in a range of applications, including smartphones and automobiles, semiconductors and microprocessors are faster, smaller and more powerful, for thermal and optical application[3]. Composite materials, along with metals and alloys, and polymeric materials, have become one of the major groups of high-performance science materials in recent years these science materials are made up of at least two different materials. An interface layer coupled to two immiscible phases matrix and reinforcement or filler binds these different materials in a ready composite. The final properties of the composite are determined by the properties of two phases, the distribution of reinforcement or filler in the matrix, and the adhesion phenomenon between the filler and the matrix. The idea of combining two

or more separate components to form a single substance opens up virtually infinite possibilities for the creation of new engineering materials a broad array of characteristics [4,5].

1.2 Polymers

Polymeric materials are among the most used materials at the present time, as polymeric materials are characterized by their cheap price, ease of manufacture, good specifications and often reach very good. It is known that most of the polymeric materials are insulating materials and that these materials have entered the electrical and electronic industries long ago. Long as an auxiliary material, but the good qualities of these materials have made polymeric materials a basic material that can be used in the electrical and electronic industries. [6] Therefore, the process of changing the electrical properties of polymeric insulating materials can be considered an important matter that can be used in the electronic and electrical industries [7].

1.2.1 Polymer Structure

Polymer science was born in the great industrial laboratories of the world of the need to make and understand new kinds of plastics, rubber, adhesives, fibers, and coatings. Only much later did polymer science come to academic life perhaps because of its origins, polymer science tends to be more interdisciplinary than most sciences, combining chemistry, chemical engineering, materials, and other fields as well [8]. Polymerization is the process of continuous connections to a chain or network structure of one or two, often more, forms of small molecules, resulting in a very large molecule with hundreds or thousands of atoms. These large molecules are classified as monomers, as the essential building blocks [9]. The size and shape of near to their properties are the polymers. The polymer form has a strong relationship with the size of the different units that make up the

macromolecules and to the different primary and secondary bonding forces that are present within the chain and between the chains [10].

1.3 Classification of Polymers

Polymers cannot be classified under one category because of their complex structures, different behaviors and vast applications. We can, therefore, classify polymers based on the following considerations.

1.3.1 Thermal Classification of Polymer

According to the effect of temperature, polymers can be classified into three types as follows:

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

b. Elastomers Polymers: Elastomers are a form of network polymer that is lightly cross linked and can be extended to extreme lengths reversibly. They have very tightly randomly coiled molecules when not stressed, which are expanded and become more ordered as they are stretched. This reduces the randomness of the chains resulting in a lower entropy in the material, and this entropy decrease is due to the retroactive force observed. When a material is extended, cross-links prevent molecules from moving past one another. The rubbers become glassy or crystal clear as they cool (partially). When heated they don't flow because of cross-links in a traditional sense. Vulcanized rubber and neoprene [12], as shown in figure (1.1.b).

c- Thermoset Polymers: These polymers have been modified chemically. when hot. When heated thermosets are typically networked polymers with a high degree of interconnection between polymer chains. These polymers are insoluble after heating, they are not heater and electric conducting and hard because their molecules are connected by strong chemical bonds. Examples of this kind of polymers are phenol formaldehyde resin and urea formaldehyde resin[12], as seen in figure. (1.1.c).

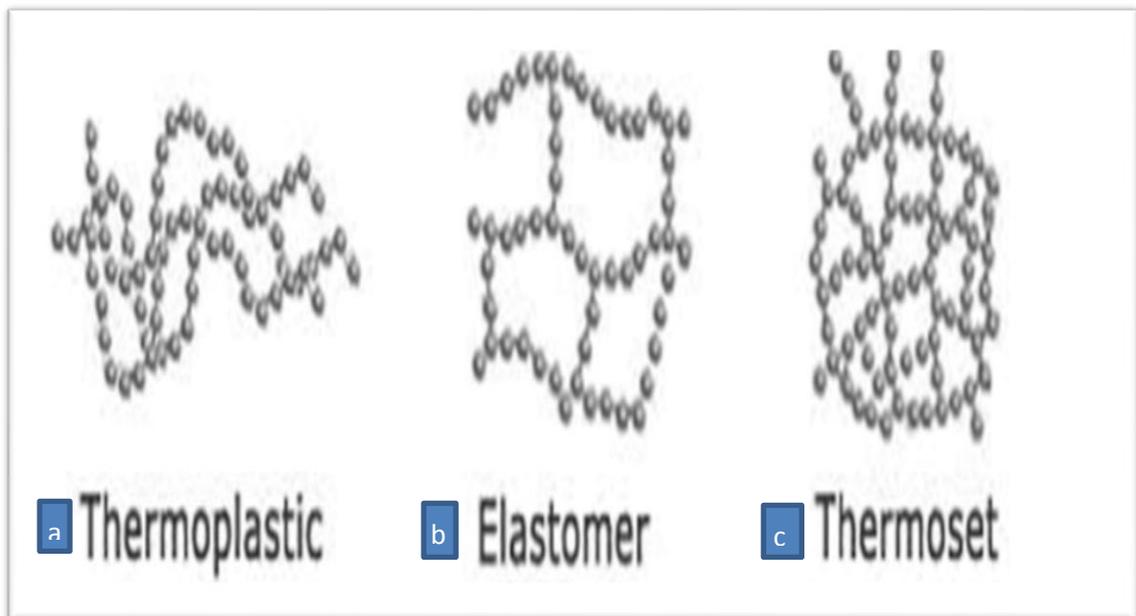


Figure (1.1): Schematic representation of (a-Thermoplastic polymer, b-Elastic polymer, c- Thermoset polymer) [13].

1.3.2 Classification Based on the Structure of the Polymers:

There are three different types based on the structure

1.Linear polymers: these polymers are linearly organized. Only a bi-functional monomer can form linear polymers. They are usually thermoplastic polymers and, except for very high molecular weight materials, are soluble in solvents. These polymers have the ability to crystallize more than other polymers and have the desired mechanical

properties. The fundamental structural unit for these polymers is a molecular sequence of a certain length linked in linear form. Polyethylene, polyvinyl chloride, polystyrene, polymethyl methacrylate, nylon, and fluorocarbons are some of the most common linear polymers [14], as shown in figure (1.2.a)

2.Branched Polymers: The reaction between polyfunctional molecules results in structural units that can be connected in such a way as to form non-linear structures. In certain situations, the side growth of each polymer chain can be stopped before the chain has a chance to link up with another chain. The resulting polymer molecules are said to be bundled. Branching can produce several physical properties in a polymer, such as a decrease in solvent solubility, a rise in the softening point and also a decrease in thermoplastic properties. For example, high density polyethylene (HDPE) is primarily a linear polymer, while low density polyethylene (LDPE) contains short chain branches [15], as shown in figure (1.2.b).

3.Cross Linked Polymers: Polymer chains, in this category are intertwined and are interconnected with more than one site, it is clear in figure (1.2.c). By covalently or ionic ally bonding polymer chains together, a network is formed that reduces molecular freedom, increases thermal resistance, and increases polymer rigidity while reducing flow properties. Chemical reactions that occur after heating create cross-linked covalent bonds. Cross-linked polymers are no longer dissolved and instead swell in the presence of a solvent (except ionic ally cross linked). A gel is a cross-linked polymer that has swollen. The degree of crosslinking has a major effect on the polymer's physical and mechanical properties. When the degree of crosslinking is increased, the rubber properties decrease and the melting point increases. When the degree of crosslinking is high, the polymer

becomes non-fusion and non-conductive to heat and electricity For example, Bakelite (used in electrical insulators), Melamine etc. [16].

4-Network polymers: polymers comprise one of the most important classes of polymeric materials,. The linking together of macromolecular chains usually through permanent covalent bonds confers unique properties to network polymers. These may be increased elasticity, solvent resistance, high temperature stability. For example Epoxies[16].

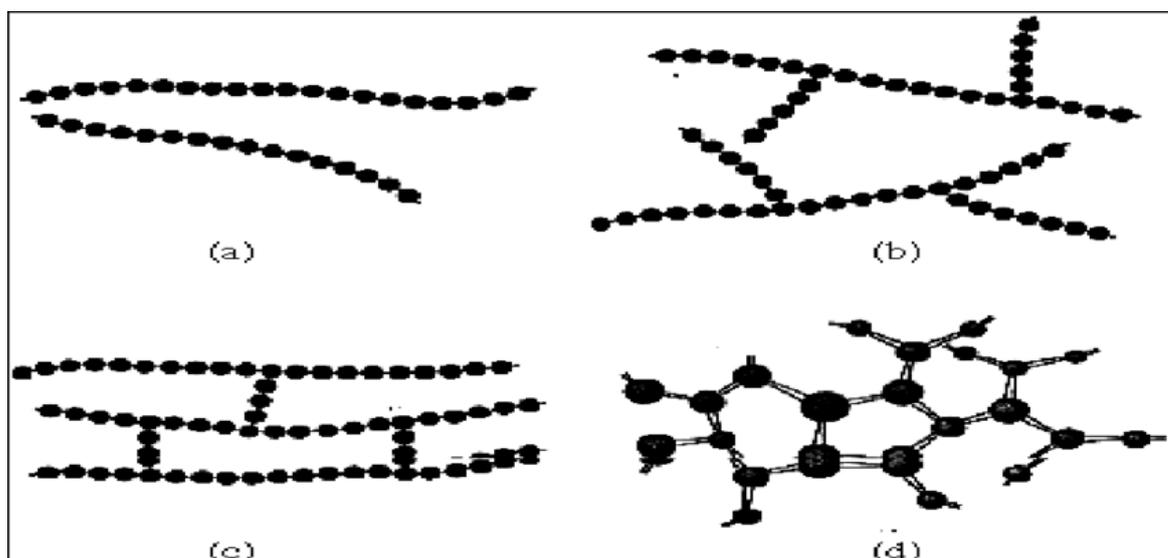


Figure (1.2): Constructivism Authority for (a- Linear polymer, b- Branched polymer, C -Cross linked polymer, d- Network polymers) [17].

1.3.3 Classification of Polymers Dependent on Homogeneousness

Polymers are classified according to the homogeneity of the repeater units.

In to: [18,19]

1- Homo polymers

Materials made from one monomer are termed homo polymers.

2-Copolymers

If their materials are made from more than one type of monomer, they have been termed copolymers

3- Composites Polymer

It is the method of introducing such materials to homogenous polymers to alter their properties and to join new recipes.

1.3.4 Classification Based on Sources Polymers

Polymers are of two primary origins: [20,21].

1- Natural Polymers:

Natural polymers There are plant or animal based compounds such as wood, cotton, natural rubber, wool, and silk. Starch, protein and cellulose are the natural foods that are natural polymers. Natural polymers may have some properties such as biocompatibility, biodegradability and low toxicity.

2- 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 colors. Synthetic polymers provide some other properties such as mechanical and physical properties and thermal stability.

1.4 Nanomaterials

One nanometer (nm) is one-billionth of a meter. These materials often have unique properties resulting from their size, shape, and chemical composition [22]. Two principal factors cause the properties of nanomaterials to differ significantly from other materials: increased relative surface area and quantum effects. Through physical and chemical processes, there are many types of nanomaterial processing accomplished to show various morphologies, including, nanorods, nanowires, nanobelts, nanocages, nanocombs, nanosaws, nanospirals, nanosprings, nanorings,

nanohelix, etc. In general, physical methods aim to address nanostructure synthesis by reducing the size of the bulk content constituents (top-down approach), whereas chemical methods aim to attempt to monitor the selection of molecules in the nanoscale range (bottom-up approach). In nanomaterial processing, there are many approaches that have been researched such as: hydrothermal method, solvothermal method, sol gel electro deposition[23].

1.5 Nanocomposites:

Nanocomposites are composites in which at least one of the phases shows materials that exhibit unusual property combinations and unique design possibilities and are thought of as the materials of the 21st century with an estimated annual growth rate of about 25% and huge demand for engineering polymers, their potential is so promising that they are useful in several applications ranging from packaging to bio-medical. Literature survey reveals that about 18,000 publications, including papers and patents, have been published on nanocomposites in the last two decades. It has been reported that at the nanoscale (below about 100 nm), a material's property can change dramatically. With only a reduction in size and no change in the substance itself, materials can exhibit new properties such as electrical conductivity, insulating behavior, elasticity, greater strength, different color and greater activity-characteristics that the very same substances do not exhibit at the micro or macro scale [25]. The general idea of nanocomposites is based on creating an extensive interface between the nanosized building blocks and the polymer matrix [26]. The mechanical, electrical, thermal, optical, electrochemical, catalytic properties of the nanocomposites will differ markedly from the component materials [27].

1.6 Applications of nanocomposites in industry:

1. Fiber/textile electrically conductive textiles, sensors, mechanical reinforcement, electromagnetic shielding, microwave, absorption, electrical energy storage (capacitors), actuators) [28].
2. Chemical sensors, pressure sensors (detection and identification of gases, including atmospheric pollutants, flammable gases, solvent vapors like Touch sensors for interaction Between operators and machines) [29].
3. Refractive index tuning (optical connectors, optical fibers and switches, signature management) [30].
4. Aerospace (Impact/damage resistant carbon fiber-reinforced polymers, transparent materials (canopies), surface coatings for signature management, corrosion protection [31].
5. Ultraviolet irradiation resistance (Components and coatings exposed to sunlight, space coatings, textiles exposed to sunlight, paint and other surface protection) [32].
6. Porous nanocomposites (Shock absorbing materials, acoustic absorbents, vehicle seat with the advantage of reduced flammability) [33].
7. Existing industrial (Functional and lightly loaded components, presently made from plastics or light alloy (handles, components of portable weapons systems, especially where injection molded plastic can replace metal components[33].
8. Ballistic protection (Body/personal armour where flexibility of movement is required, in particular protection against blunt weapons (stones, sticks and bars for arms and legs [34].

9-Inorganic antimicrobial compounds metal salts, nanoparticle-sized metals, and metal oxides appear promising. CuO, TiO₂, ZnO, Al₂O₃, SiO₂, Fe₂O₃, and CeO₂ are frequently utilized as antibacterial agents in metal oxides[34].

1.7 Materials used in the Study

1.7.1 Polyvinyl alcohol (PVA)

The chemical formula of poly vinyl alcohol (PVA) $[(CH_2CH(OH))_n]$ and it is a polymer with exceptional properties such as water solubility, biodegradability, biocompatibility, non-toxicity, and non-carcinogenic that possesses the capability to form hydrogels by chemical or physical methods [35]. PVA has high enough tensile strength and satisfactory flexibility. To improve deformability PVA is usually plasticized by the variety of low molecular compounds mostly containing polar groups [36], which associate with hydroxyl groups of PVA chain (with or without water assistance) developing hydrogen bonds, thus reducing direct hydrogen bonding between PVA macromolecules [37]. The comparatively high biodegradability in the environment may be one of the most important and desirable characteristic of PVA, because the polyvinyl type polymer consisting of a carbon-carbon main chain is scarcely biodegradable [38]. This property of PVA has been reevaluated recently, and much effort has been made to produce PVA-based biodegradable polymeric materials having preferred physical and chemical properties for use in industrial and medical fields [39]. Table (1.1) shows to physical properties of (PVA).

Table (1.1): The physical Properties of PVA polymer [40]

<i>Physical properties</i>	<i>Units</i>	<i>Results</i>
Molecular weight	g/mol	150000
Solution PH		5 -7
Density	g/cm ³	1.19-1.31
Specific volume	m ³ /kg	7.7 x 10 ⁻⁴
Specific heat	J/kg·K	1674
Meltingpoint (unplasticized)	°C	230 for fully hydrolyzed grades, 180-190 for partially hydrolyzed grades
Tg	°C	75-85
Electrical hconductivity	(Ohm.c m) ⁻¹	1*10 ⁻¹³
Stability to sunlight		Excellent

1.7.2 Barium Titanate (BaTiO₃)

Barium titanate (BaTiO₃) belongs to the perovskite family, which includes a significant number of compounds with the general formula (ABO₃), where A denotes a divalent cation and B denotes a tetravalent cation. It is one of the most popular electronic ceramic components in use for over 60 years. This is due to its favorable characteristics, which include: first, its comparatively clear crystal structure, second, its ability to exhibit ferroelectric properties at room temperature, and finally, its ease of preparation as polycrystalline ceramic. Because of its high dielectric constant, barium titanate is a popular material for capacitors. It can also be

used for medical imaging, gas lighters, ultrasonic ventilation, and underwater detection, among other things [41-43]. Barium titanate has been used in several different applications, some of which are described below:

1-The capacitor: A capacitor is an electrical device that can store electrical energy and is made up of two conducting plates (usually made of metal) separated by a dielectric (insulating) material [44].

2- The gas lighter: As a mechanical stress is applied to a piezoelectric cylinder, a high voltage is generated between two closely separated electrodes, which is high enough to cause air breakdown between the electrodes, resulting in a spark, which, when exposed to combustible gas, ignites it to produce flame.

3-The ultrasonic cleaning: The item to be cleaned is placed in a stainless steel tank containing an appropriate solution, the electrical energy from the power source is converted to ultrasonic waves by the piezoelectric transducers, and the item to be cleaned is extracted contaminants from sections immersed in aqueous media by using high-frequency sound waves (above the upper limit of human hearing). (Which are placed in the bottom or sides of the stainless steel tank), the ultrasound wave generates bubbles in the liquid medium, which implode as they reach a certain level, releasing high energy, which is used to dissolve the grime [45].

4-Ultrasound in medicine: Medical ultrasound is a form of medical imaging that uses sound waves to see into the body. A piezoelectric transducer encased in a probe generates the ultrasound pulse, which vibrates and produces the ultrasound wave as an electrical pulse is applied to it , When these waves enter the body, some of them will be reflected back into the probe, causing the probe to produce electrical pulses. The system then processes these electrical pulses and creates an image .

5- The detection in the water: A transduce (piezoelectric element) receives a periodic of electrical signals to enable it to send a pocket of ultrasound wave into the water, allowing it to generate electrical signals as the waves emitted from the target return to the transduce. Since the speed of sound in water is known, the time it takes for the waves to return to the transducercan be calculated, the distance to the reflected source can be calculated from it [46].

1.7.3 Titanium Dioxide (TiO₂)

Titanium dioxide, also known as Titanium (IV) oxide or Tatiana [47], is the naturally occurring oxide of titanium, chemical formula TiO₂. When Titanium dioxide occurs in nature as the well-known naturally occurring minerals rutile, anatase and brookite. The most common form is rutile, which is also the most stable form. Anatase and brookite both can be converted to rutile upon heating. Rutile, anatase and brookite all contain six coordinates titanium, because of its brightness and very high refractive index (n=2.609), in which it is surpassed only by a few other materials. [48].When deposited as a thin film, its refractive index and color make it an excellent reflective optical coating for dielectric mirrors .TiO₂ is extensively used in gas sensing because of its desirable sensitivity and mainly because of its good stability in adverse environments. Titanium (IV) oxide (II) has one stable phase, rutile (tetragonal) and two metastable polymorph phases, brookite (orthorhombic) and anatase (tetragonal). It has wide application value in many fields due to its excellent structural, optical, and chemical properties[48]. Table (1.2) shows the physical and chemical properties of the TiO₂ structures.

Table (1.2): Physical and chemical properties of the three TiO₂ structures[48].

Properties	Rutile
Molecular_formula	TiO ₂
<u>Molar mass</u>	79.866 g/mol
Crystal System	Tetragonal
Energy gap Eg	3.06 ev
Color	White solid
Density	4.27 g/cm ³
Melting_point	1855C°
Boiling point	2972 C°
Refractive_index (n_D)	2.609
Dielectric constant ε	110~117
Hardness(Mohscale)	7.0~7.5

1.8 Literature Review:

1-In (2013), M.H. Al-Humairi [49] studied the optical and electrical properties of (PVA/Ag) and (PVA/TiO₂) nanocomposites .He found that the absorbance, absorption coefficient, extinction coefficient, refractive index and dielectric constant (real, imaginary), D.C electrical conductivity, dielectric constant, dielectric loss, and the A.C electrical conductivity are increasing with increasing concentrations of the (Ag,TiO₂) nanoparticles but the energy gap and activation energy are decreasing with the increasing of concentrations of the (Ag,TiO₂) nanoparticles and the dielectric constant and the dielectric loss are decreasing with the increase of frequency, but the A.C electrical conductivity of nanocomposites is increasing with increasing of the frequency .

2-In (2014) ,S.Sugumaran *et al* [50] studied the transparent nanocomposite PVA–TiO₂ and PMMA–TiO₂ thin films. Optical and dielectric properties were prepared by simple and cost effective dip coating method. He found the SEM analysis showed cluster of TiO₂ nanoparticles were well dispersed in the polymer matrix. Both nanocomposite films have a transmittance of >80% in the entire UV–Vis–NIR region. Optical properties showed very high transmittance, wide band gap, low absorption coefficient, low extinction coefficient and high refractive index. The optical band gap energy was found to be about 3.77 eV and 3.78 eV respectively for nanocomposite PVA–TiO₂ and PMMA–TiO₂ thin films. Very good dielectric behavior like high dielectric constant, low values of dielectric loss .

3-In (2014) M.A.Habeeb *et al* .[51] studied the dielectric properties of PVA-TiO₂ composites. He conclude that dielectric constant, dielectric loss and electrical conductivity are increasing with the increase of the concentration of the titanium dioxide. Also the dielectric properties (dielectric constant, dielectric loss and electrical conductivity) changed with the increase of the frequency.

4-In (2016) S. A. Madhloom *et al*. [52] studied the structural properties of nanoparticles TiO₂/PVA Polymeric films ,will be used casting method is used to prepare homogeneous films on glass petri dishes. The SEM showed crystalline structure of TiO₂ nanoparticles and matching with XRD results, the SEM image of TiO₂ /PVA films showed rough surface with some gathering of PVA polymer.

5-In (2016) A.M.Shehap *et al*.[53] studied the structural and optical properties of TiO₂ nanoparticles/PVA for different composites thin films . The structural properties of those samples were examined by XRD, FTIR, and UV-Visible. The absorption spectra of UV-Visible light showed

irregular changes of the absorption for high doping samples in UV range (7.5, 10 TiO₂ /PVA). Absorbance, transmittance and reflectance spectra were used for the determination of the optical constants. The results indicated that the optical band gap decreases with increasing TiO₂ content, while the refractive index increased to high value for the composites of high dopant.

6- In (2017), R. G. Kadhim *et al.* [54] studied the nanocomposites with varying concentrations of (poly vinyl alcohol – carboxy methyl cellulose – copper oxide), the electrical conductivity and dielectric constant were examined. According to the results, the electrical conductivity of the (PVA-CMC) blend increases as the copper oxide nanoparticle concentrations grow at 100Hz, while the dielectric constant and dielectric loss decrease as the frequency rises.

7-In (2018) S. Ningaraju *et al* [55] studies the free volume controlled electrical properties of PVA/NiO and PVA/TiO₂ polymer nanocomposites. The Scanning Electron Microscopy (SEM) studies demonstrate the formation of nanoclusters by the agglomeration of nanoparticles at higher wt% of nanofiller loading. The increased AC/DC conductivity of PVA/NiO and at lower concentration of TiO₂ in PVA/TiO₂ polymer nanocomposites suggests the increased mobility of ions and electric charge carriers. The decreased conductivity at higher concentration of TiO₂ indicates the reduced conducting pathways for the mobility of ions and electric charge carriers due to the increased ion aggregation. The increased dielectric constant and dielectric loss up to 0.1 wt% of NiO and 0.4 wt% of TiO₂ suggests the increased dipole polarization. The decreased dielectric constant after 0.4 wt% of TiO₂ is attributed to the reduced dipole polarization by the formation of thin immobile nano-layers and hence the polymeric chain mobility.

8-In (2019), K Chidambaram *et al* [56] studied the influence of hexagonal boron nitride and BaTiO₃ as hybrid Fillers on the structural, morphological and dielectric behavior of polyvinyl alcohol nanocomposites. The mechanical properties found some enhancement in the thermal stability for this polymer nanocomposites, in this polymer nanocomposites the dielectric constant can be tuned, and can be used in thin film transistors, organic printed circuit boards or in embedded dielectric components.

9-In (2020), S.Lssa *et al.*[57] studied the structure and optical properties of (PVA–BaTiO₃) nanocomposite films. This results showed that BaTiO₃ content increases in the polymer matrix, transmission decreases .The absorbance, absorption coefficient, extinction coefficient, refractive index and dielectric constant (real, imaginary)increases with increases BaTiO₃ content. The energy gap decrease with the increase of concentrations of BaTiO₃.

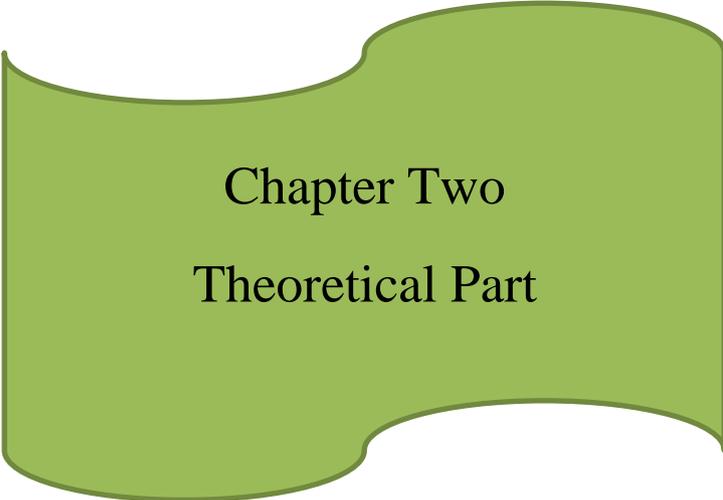
10-In (2020) Q. Jebur, *et al.* [58] studied the structural and dielectric properties of(PVA-PEO-Fe₂O₃) nanocomposites. The dielectric constant and dielectric loss are decreased while the electrical conductivity increases with the increase in the frequency of the applied electric field. The optical measurements showed the absorbance of (PVA-PEO-Fe₂O₃) nanocomposites is increased with the increase of the concentrations of iron oxide nanoparticles. The indirect energy gap(E_g) of (PVA-PEO) blend decreases with the increase of the concentrations of iron oxide nanoparticles. The optical constants such as absorption coefficient, extinction coefficient, refractive index, real, and imaginary dielectric constants and optical conductivity of (PVA-PEO) blend varied with the increase of the weight percentages of iron oxide nanoparticles.

11-In (2021) ,T.S.Soliman *et al* [59] studied the structure and optical properties of(PVA - BaTiO₃) nanocomposite. The enhancement in structural and optical properties of(PVA - BaTiO₃) nanocomposite. The absorbance and optical constants of (PVA-BaTiO₃) nanocomposite increases with increase concentrations of BaTiO₃ nanoparticles. The energy band gap decreases with increasing concentrations of BaTiO₃ nanoparticles.

12-In (2021), B. Mohammed *et al* [60] studied the influence of BaTiO₃ NPs on dielectric characteristics of PVA/PEG for electronic applications. The dielectric parameters of PVA/PEG were found to be improved with increasing BaTiO₃ NPs contents and the dielectric parameters changed with increasing the frequency. Moreover the dielectric constant was increased from 5.8 to 8.6 and the dielectric loss was increased from 1.5 to 4.38 The ϵ' and ϵ'' were decreased from 8.34 to 2.40 while the electrical conductivity was increased at 4.38 HZ. The σ_{AC} was decreased with rising the frequency. The obtained results showed the PVA/PEG/BaTiO₃ nanostructures have many applications in electrical and electronic fields .

1.9 The Aims of the Study

1. Preparation of(PVA-BaTiO₃-TiO₂) nanocomposites.
2. Study of structural, optical and dielectrical properties of (PVA-BaTiO₃-TiO₂) nanocomposites.
3. Application of (PVA-BaTiO₃-TiO₂) nanocomposites for antibacterial



Chapter Two
Theoretical Part

2.1 Introduction

This chapter provides an general idea of the study theoretical component, which contains physical ideas, scientific classifications, correlations, and the laws used to explain the study's findings.

2.2 Optical Properties

The size dependent properties of electrons result in significant variations in the optical properties of nanoscale materials. Quantum effects occur when particles are reduced sufficiently small, limiting the energies at which electrons and holes can be invested in these particles, as energy is proportional to wavelength. This enables the particle's optical characteristics to be fine-tuned in respect to its size. Thus, by merely altering the size of particles, they may be made to emit or absorb specific wavelengths of light [60]. Understanding a polymer's absorption and transmission spectra enables the identification of certain optical properties across a variety of wavelengths. A UV test enables us to determine the shape of the linkages, orbital beams, and energy beams. The examination of the visible application spectrum reveals a wealth of information about solar application activities. To determine the overall structure of a polymer and its chemical structure, infrared examination is required [61].

2.2.1 Absorbance (A)

The ratio of the material's absorbed light intensity (I_A) to its incident light intensity (I_o) can be measured using absorbance [62]:

$$A=I_A/I_o \dots\dots\dots (2.1)$$

2.2.2 Transmittance (T_r)

(I_{Tr}) This ratio for the film's transmitted rays' intensity (I_{Tr}) to the incident rays' intensity (I_o) is as follows [63]:

$$T_r = I_{Tr}/I_o \dots\dots\dots (2.2)$$

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 [64]. The regions of absorption can be divided into three distinct regions [65]:

A) Region of High Absorption

This area is depicted in Figure (2.1). The magnitude of the absorbent coefficient (α) in section (A) is larger than or equal to (10^4 cm^{-1}). This could involve an optical energy gap that is prohibited. (E_g^{opt}).

B) Exponential Region

As displayed in Figure (2.1), this area component (B) is equivalent to ($1 \text{ cm}^{-1} < \alpha < 10^4 \text{ cm}^{-1}$) for the absorption coefficient (α). It represents the conversion of extended levels in the conductive band (C.B.) to local levels in the conductive band (C.B.) from the Valens band (V.B.).

C) Low Absorption Region

The figure depicts this Figure (2.1). Part (C) has an extremely low absorption coefficient, around ($\alpha < 1 \text{ cm}^{-1}$). The transition occurs in this area as a result of defects in the state density of space movement.

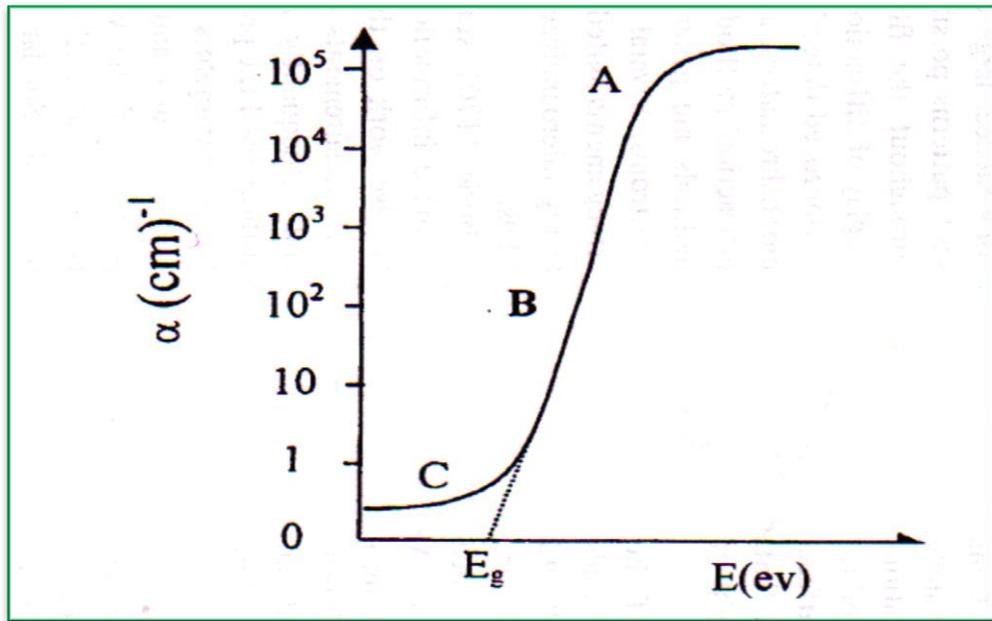


Figure (2.1): The difference of absorption edge with absorption regions [65].

2.2.4 The Electronic Transitions

Electronic transformations are broadly divided into two groups [66]:

1. Direct transition

In semiconductors, this transformation occurs when the (C.B) base is exactly above the top (V.B). This implies that the wave vector has the same value ($K=0$). The absorption occurs in this condition ($h\nu=E_g^{opt}$). This form of transition calls for energy and momentum conservation laws. There are two forms for direct transitions. [67]

a) Direct allowed transition: It occurs from the top (V.B) points and the bottom (C.B), as seen in the figure (2.2-a).

b) Direct forbidden transitions: As given in this figure (2.2-b), this transition occurs between the close high points of (V.B) and the lower points of (C.B) [68]. For this transition form, the absorption coefficient is indicated:

$$\alpha h\nu = B (h\nu - E_g^{opt})^r \dots\dots\dots (2.3)$$

Where: E_g^{opt} : energy gap between direct transition.

α : is the absorption coefficient.

B: constant depended on type of material.

h: is the Planck's constant.

ν : is the photon frequency.

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. This kind of transformation occurs with the beneficial "Phonon" particle for energy conservation and energy law. Two kinds of indirect transitions exist [64], they are:

c) Allowed indirect transitions:

These transitions occur between the top of the (V.B.) and the bottom of (k-space), as shown in figure (2.2-c) (C.B.).

d) Forbidden indirect transitions

As shown in the figure, such transitions occur between points near the top of (V.B.) and points near the bottom of (C.B) [65]. (2.2-d). The coefficient of transition absorption is denoted by Phonon on absorption:

$$ah\nu = B(h\nu - E_g^{\text{opt}} \pm E_{\text{ph}})^r \dots\dots\dots (2.4)$$

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

($r = 2$) for the allowed indirect transitions

($r = 3$) for the forbidden indirect transitions

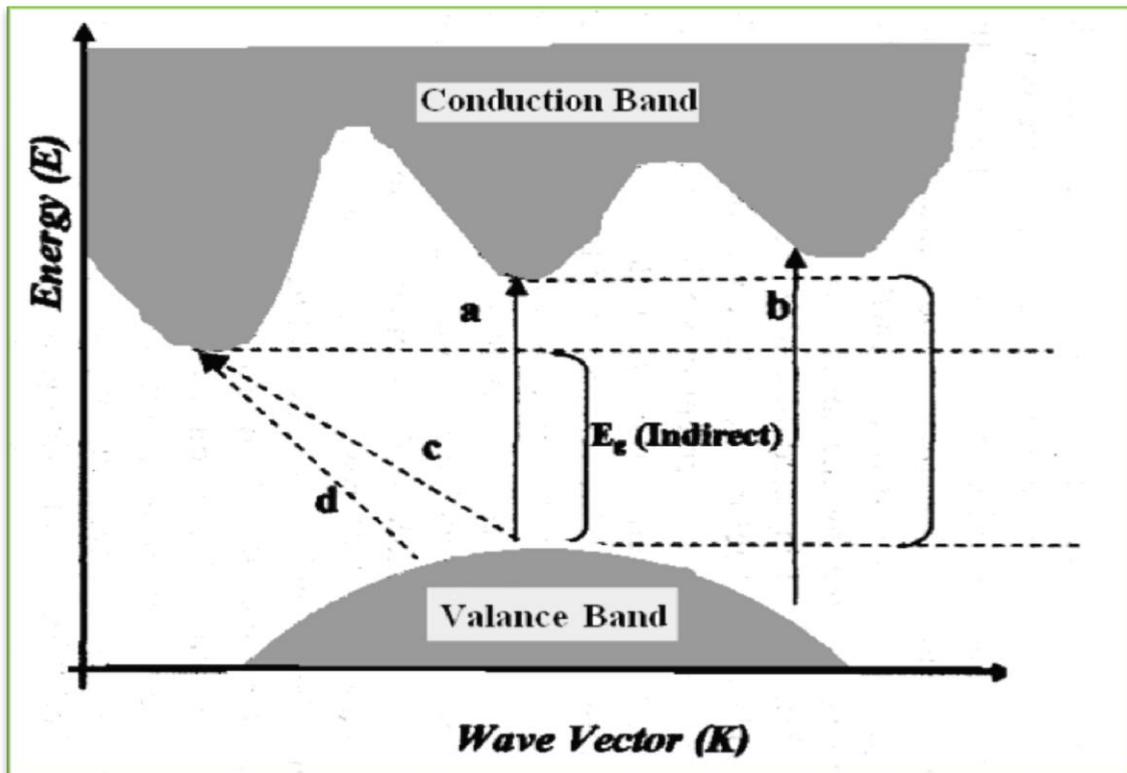


Figure. (2.2): The transition types [66]

- a) Allowed direct transitions. (b) Forbidden direct transitions.
 (c) Allowed indirect transitions. (d) Forbidden indirect transitions.

2.2.5 Optical Constants

The study of a material's optical constants is fascinating for a variety of reasons. To begin, materials used in optical applications such as interference filters, optical fibers, and reflective coatings require an accurate understanding of their optical constants throughout a broad range of wavelengths. Second, all

materials have optical properties that are related to their atomic structure, electronic band structure, and electrical properties [67].

2.2.5.1. Absorption Coefficient (α)

The absorption coefficient (α) is defined in the direction of wave diffusion in the medium as the gradual reduction of incident energy flow in an incident field. The coefficient of absorption depends on the photon energy and properties of the semiconductor for gap energy and electronic transitions [68]. The relationship between incident (I_0) and penetrating (I) is defined in the following equation beer- lambert as being related to the absorption of light. [69]:

$$I = I_0 e^{-\alpha t} \dots\dots\dots(2.5)$$

where (t) is the matter's thickness and (α) is the absorption coefficient, which is measured by cm^{-1} .

$$\alpha t = 2.303 \log I/I_0 \dots\dots\dots(2.6)$$

where the $\log I/I_0$ value denotes the absorbance (A). This is how the absorption coefficient is determined [70]:

$$\alpha = 2.303(A/t) \dots\dots\dots (2.7)$$

2.2.5.2. Refractive index (n)

Speed of light in a vacuum to the speed of light in a medium is known as the reflectance . It is also possible to define reflection as the ratio of the incident rays reflection to the reflection at the boundary between two media, which is what we call the reflectance (R). The following equation [71] illustrates the relationship between reflectivity and refractive index:

$$R = (n-1)^2 + k^2 / (n+1)^2 + k^2 \dots\dots\dots (2.8)$$

(k) denotes the extinction coefficient.

Additionally, the absorbance (A) and transmittance (T) can be determined using the given equation [71]:

$$R + A + T = 1 \dots\dots\dots (2.9)$$

Refractive index can be expressed by the given equation [71]:

$$n = \sqrt{\frac{4R-k^2}{(R-1)^2} - \frac{(R+1)}{(R-1)}} \dots\dots\dots (2.10)$$

2.2.5.3. Coefficient of extinction (k_0)

Coefficient of extinction : define attenuation in the intensity of electromagnetic radiation It is a fictitious part of a complex index of refraction. (n) [72]:

$$N=n-ik_0 \dots\dots\dots(2.11)$$

n: the real part of the refractive index

N: is a complex refractive index that is dependent on the material type, crystal structure (grain size), crystal defects, crystal stress, and extinction coefficient (k_0) [73].

$$k_0 = \frac{\alpha\lambda}{4\pi} \dots\dots\dots (2.12)$$

λ : is the photon ray wavelength.

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. [74]. By the following equation, the real and imaginary dielectric constant can be determined [75]:

$$\varepsilon = \varepsilon_1 - i\varepsilon_2 \dots\dots\dots(2.13)$$

where: ε is the complex dielectric constant and $(\varepsilon_1, i\varepsilon_2)$ are the imaginary and real parts of the dielectric constant, respectively. The dielectric constant's real and imaginary components are connected to and values.

$$\varepsilon = N^2 \dots\dots\dots(2.14)$$

$$(n - ik_0)^2 = \varepsilon_1 - i\varepsilon_2 \dots\dots\dots (2.15)$$

From equation (2.13) real and imaginary dielectric constant can be written as follows:

$$\varepsilon_1 = (n^2 - k_0^2) \dots\dots\dots (2.16)$$

$$\varepsilon_2 = (2n k_0) \dots\dots\dots(2.17)$$

2.2.5.5 Optical Conductivity (σ_{op})

The optical conductivity (σ_{op}) depends directing on the refractive index (n) and absorption coefficient (α), according to the following relation [76]:

$$\sigma_{op} = \frac{\alpha n c}{4\pi} \dots\dots\dots (2.18)$$

c : is the velocity of light, α is the absorption coefficient.

2.3 Electrical Properties

Electricity is the movement of charged units, which have the influence of possible differences, called carriers. These units are solid state electrons of matter or liquid and gas ions. Given the transfer of electricity to solid matter by electron movement, the electrical properties of the matter are predicted to depend essentially on their electronic configuration. [77,78]. The subjects are categorized by their electric conductivity to:

1-Isolators: their conductivity extends from 10^{-22} – 10^{-8} (ohm .cm)⁻¹

2-Conductivities range from semiconductors 10^{-8} – 10^{-3} (ohm.cm)⁻¹

3-Leaders (metals): more than their conductivity 10^{-3} (ohm .cm)⁻¹

4-Things of super conduct: its conductivity is 10^{20} (ohm .cm)⁻¹.

To understand the electrical properties of more about the levels of energy and electronic delivery and how electrical conductivity is carried out at these levels is significant. Electron in a nuclear is distributed at various energy levels electrons closest to the core are bound more closely to the atom and electrons are less connected to the core. Electrons are farther away from the core. Electrons which are the most far from the nucleus are also the least related to the nucleus. These electrons are known as electrons of valence. The electrons of valence are divided between several levels of energy known as valence bands. [75,79].

2.3.1 Electrical Conduction

Electric conductivity is described as the process of transferring the electric charge from an electric field to another position in the medium. Two primary factors are involved. The first is the load carrier (n), the second is the carriers' kinetic susceptibility (μ) [80]. It is subject to temperature (T) and the potential applied(V).

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 [81]:

$$\mu_j = p E_i \dots\dots\dots (2.19)$$

Where μ_i is the electric dipole moment, p is the atom or molecule's polarity and E_i is a molecule internal field, proportional to the external field. Thus, for the unit length, the complete dipole moment (P):

$$P = N_o \mu_i \dots\dots\dots(2.20)$$

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 [81]:

$$P = D - \epsilon_o E \dots\dots\dots(2.21)$$

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

$$D = P + \epsilon_o E = \epsilon_o \epsilon' E \dots\dots\dots (2.22)$$

As

$$\therefore \epsilon' = D / \epsilon_o E \dots\dots\dots(2.23)$$

$$\therefore \epsilon' = 1 + \frac{P}{\epsilon_o E} \dots\dots\dots(2.24)$$

Where ϵ' Dielectric constant. The balance of a volume unit's relative dielectric constant and polarity indicates the connection with Clausen Rossetti. [82]

$$N_o P / 3 \epsilon_o = \epsilon' - 1 / \epsilon' + 2 \dots\dots\dots (2.25)$$

This equation can be applied to the electric insulators ionic and non-polar.

2.3.3 Mechanism of Polarization

The components of the polarization can be defined by polarizing of substances

to demonstrate the form of total polarization figure (2.4) polarization mechanism [82]:

$$P_{\text{total}} = P_e + P_d + P_o + P_i \dots\dots\dots(2.26)$$

A- Electronic Polarization (P_e)

The charge distribution is distorted by an external electrical field as given in figure(2.4-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 [83,84].

B- Ionic Polarization (P_i)

Ionic bonding materials can be ionic polarized. Ion polarization is the shift in positive and negative electrodes, as seen in the figure (2.4-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 [85].

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. [86], like in figure (2.4-c).

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

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 (2.4-d) [87].

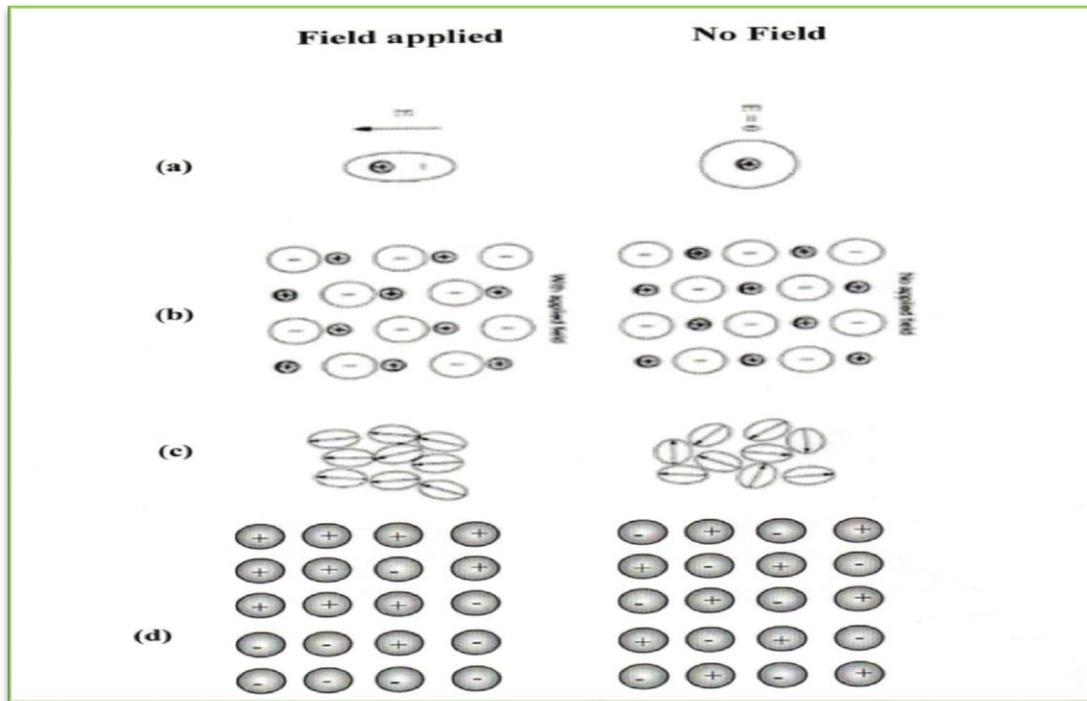


Figure (2.3): The four types of polarization [88].

a-Electronic polarization.

b-Ionic polarization.

c-Orientation polarization.

d-Space charge polarization.

2.3.4 The A.C Electrical Conductivity

As an alternative to the D.C conductivity test, A.C techniques are used and calculations are made over a broad range of frequencies. The A.C can typically be derived from the D.C conductivity value. The theory of A.C studies is the ability to provide information about the polarization response of the studied device and information on electrode capacity, resistance and capacity of the grains borders and the present level of electronic conductivity [89]. The dielectric constant is defined as the ratio of an insulating material's capacitance to its resistance used in a capacitor between its panels to the same dimensions with a vacuum between the panels. When an alternating potential

$V = V_m e^{j\omega t}$ the present passing through the condenser takes place through a condenser C filled with an insulator, preceding the capacitor by a $\pi/2$ level [90]:

$$I = j \omega C V \dots\dots\dots(2.27)$$

Where ω denotes the applied field's corner frequency ($\omega = 2\pi f$), j is imaginary number $j = \sqrt{-1}$ and V_m is the voltage maximum .

The angle between I and V was shown experimentally to be less than $\pi/2$.This emphasizes the fact that the electric stream is the sum of the I_p steering current, which is in phase with V and I_q , is expressed by the equation with a phase difference of $\pi/2$, i.e. [88]:

$$I = I_p + jI_q \dots\dots\dots (2.28)$$

The capacity of a condenser built of two parallel plates is indicated

$$C = \epsilon_0 \epsilon' \frac{A}{t} \dots\dots\dots(2.29)$$

By substituting equation (2.29) in (2.27), get:

$$I = j \omega \epsilon_0 \epsilon' \frac{VA}{t} \dots\dots\dots(2.30)$$

The permittiveness (ϵ) has to be a complex amount, the power supply is a complex quantity, as described in the equation, since it is made up of real and imaginary components (2.28). That is what we are talking about. [84]:

$$\epsilon = \epsilon' - j \epsilon'' \dots\dots\dots (2.31)$$

Where, ϵ'' The depletion of dielectric.

So, ge

$$I = j \omega \epsilon_0 \frac{A}{t} (\epsilon' - j \epsilon'') V \dots\dots\dots(2.32)$$

Equation comparison (2.32) with (2.28), then:

$$I_p = \omega \epsilon_0 \epsilon'' \frac{A}{t} V \dots\dots\dots(2.33)$$

$$I_q = W \epsilon \epsilon_0 \frac{A}{t} V \dots\dots\dots (2.34)$$

Fig (2.5-B) displays that the loss factor(tanδ) is:

$$\text{Tan}\delta = \frac{I_p}{I_q} = \frac{\epsilon''}{\epsilon'} \dots\dots\dots(2.35)$$

The depletion of dielectric this reflects the energy lost in the insulator, which is converted into thermal energy. It is very useful in electrical applications to determine the power factor. Excessive power factor will result in a heat loss in the high frequency isolator.

The condenser (c) can be defined by an ideal condenser that is connected to the low frequency resistance R_p So:

$$I_p = I_p + j I_q = \frac{V}{R_p} + j W C_p V \dots\dots\dots (2.36)$$

Get the impedance, therefore:

$$\frac{1}{Z} = \frac{1}{R_p} + j W C_p \dots\dots\dots (2.37)$$

From equations (2.33), (2.34), and (2.36), one can write:

$$R_p = \frac{t}{W \epsilon'' A \epsilon_0} \dots\dots\dots (2.38)$$

$$\epsilon'' = \frac{1}{w R_p C_0} \dots\dots\dots (2.39)$$

$$C_p = \frac{\epsilon_0 \epsilon' A}{t} \dots\dots\dots (2.40)$$

$$\epsilon' = \frac{C_p}{C_0} \dots\dots\dots (2.41)$$

Dissipated power in the insulator is demonstrated by alternative capacity as a function of the conductivity of the alternative by equality (2.40):

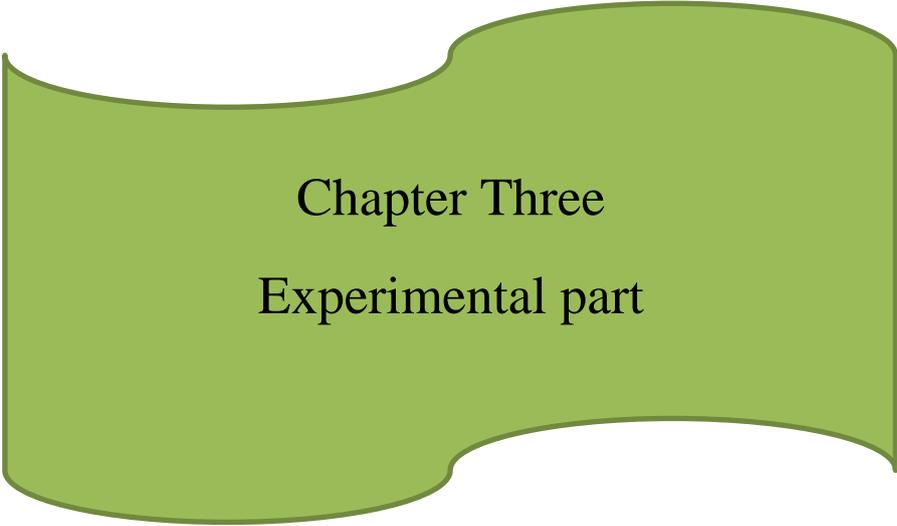
$$\sigma_{a.c} = W \epsilon'' \epsilon_0 \dots\dots\dots (2.42)$$

$\sigma_{a.c}$ The induced temperatures in the protecting material caused by the variation for this dipole in its place are measured using field alternation [91].

2.4 Anti-Bacterial Activity

Antibacterial drugs are required to inhibit germ growth while also minimizing their detrimental effects on our lives. Today, inorganic antimicrobial compounds such as metal salts, nanoparticle-sized metals, and metal oxides appear promising. CuO, TiO₂, ZnO, Al₂O₃, SiO₂, Fe₂O₃, and CeO₂ are frequently utilized as antibacterial agents in metal oxides [92]. In general, both gram-positive and gram-negative bacterial strains are considered to be a significant public health threat. Antibiotics have been used to treat infections caused by both community and hospital-acquired pathogens for many years [93].

Nanoparticles' characteristics can easily be adjusted by lowering or modifying their size, particularly when nanometer-scale alterations are used [94,95]. The widespread use of antibiotics in the prevention and treatment of bacterial illnesses has resulted in the growth of resistant germs, necessitating the development of novel antibacterial active compounds. Nanoparticles are between biological micromolecules and human cells in size. The development of nanotreatment techniques has the potential to significantly improve medical therapies [96].



Chapter Three
Experimental part

3.1 Introduction

This chapter includes the preparation process, devices and measurement techniques. A general description of materials (Polyvinyl alcohol, Barium titanate and Titanium dioxide used in this work are given by (Fourier Transform Infrared Rays(FTIR), Scanning Electron Microscope (SEM), optical properties measurements, measurement dialectical properties and includes diagrams of some electrical circuits, as well as antibacterial application

3.2 Materials used in this investigation

The materials used in this study are:

3.2.1 Matrix Material

3.2.1.1 Polyvinyl alcohol (PVA)

The material Polyvinyl alcohol (PVA) used is a white powder, the molecular weight is 150000 g/mol and could be obtained from local markets, and high purity (99.9%).

3.2.2 Additive Nanomaterial

3.2.2.1 Barium Titanate (BaTiO₃)

It was obtained as powder from local markets with density 6.02gm/cm³ from a company US Research nanomaterials, Inc. and high purity and the furrow volume of it barium titanate Nano powder (BaTiO₃, 99.9%, 50 nm, Cubic).

3.2.2.2 Titanium Dioxide (TiO₂)

It was obtained as powder from (Nano shel USA) company. With grain size (20nm) and high purity (99.9%). Nanomaterials(TiO₂) are tested by using the

apparatus (Bettersize2000 laser particle size analyzer) existed in Babylon University / College of Material Engineering, department of Electro -chemical, and the results we have come up with are within the nanomaterials description, the materials were (TiO_2).

3.3 Preparation of (PVA-BaTiO₃-TiO₂) Nanocomposite

The (PVA-BaTiO₃-TiO₂) Nanocomposites are preparation in 40 ml distilled water with a magnetic stirrer to achieve a more homogeneous solution at a temperature of 150 C°. BaTiO₃ and TiO₂ nanoparticles were added with concentrations (0,1,1.5,2 and 2.5) wt% get the films from this mixture using the casting process, which involves placing the mixture in a template (Petri dish) (with a diameter of 5cm), allowing it to dry, and then quietly removing it from the template to perform the required tests.

3.4 Measurements of Structural Properties

3.4.1 Optical Microscope

The optical microscope supplied by Olympus name (Toup View) model (Nikon-73346) as shown in figure (3.1) and fitted with a light intensity automatic operated camera is used to analyze the sample of (PVA-BaTiO₃-TiO₂) nanocomposites. This calculation was carried out Department of Physics, University of Babylon/College of Education for Pure Sciences, under magnification(10x).



Figure (3.1): Optical Microscope

3.4.2 FTIR Spectral Characterization

FTIR spectra were recorded by FTIR (Bruker company, German origin, type vertex -70). FTIR was implemented in the University of Babylon /College of Education for Pure Sciences/Department of Physics. In this study, the considered wave number range is $(500-4000) \text{ cm}^{-1}$, as shown in figure (3.2)



figure (3.2) : Fourier transform infrared (FTIR) spectroscopy device .

3.4.3 Scanning Electron Microscope

The scanning electron microscope (SEM) is an electron microscope that images the sample surface by scanning it with a high -energy beam of electrons in a raster scan pattern. The specimens for an SEM testing must be electrically conductive, at least at the surface, and electrically grounded to prevent the accumulation of electrostatic charge at the surface. Small part of (1cm²) was taken from the sample to examine it by SEM. In this work low vacuum scanning electron microscope was used. The surface morphology of (PVA-BaTiO₃-TiO₂) nanocomposites was observed using Tescan mira3 SEM microscope. is equipped with dual Bruker XFlash EDS detectors and Bruker eFlash HD EBSD (Czech Tescan Instrument Co.) for analytical studies at the University of Tehran as shown in figure (3.3). The advantage was observed using this technique (Low vacuum SE detecto) is beam deceleration technology (BDT) for high resolution

imaging and high surface sensitivity at very low kv and variable pressure operation, Fully integrated active anti-vibration system.



Figure (3.3): Image of system of SEM device.

3.5 Optical Properties Measurements

At the University of Babylon, Department of Physics, College of Education for Pure Sciences, the absorption spectrum of (PVA-BaTiO₃-TiO₂) nanocomposites films was measured with a double beam spectrophotometer (Shimadzu model UV-1800 Ao (JAPAN) in the wavelength range (190-1100) nm. As shown in figure (3.4). It found at room temperature, the absorption spectrum was recorded. The optical constants, absorption coefficient, extinction coefficient, refractive index, and energy gaps are all examples of parameters were calculated using a computer program.



Figure (3.4): Image of UV spectrophotometer (photometer).

3.6 A.C. Electrical Properties Measurement

LCR meter style (HIOKI 3532-50 LCR Hi TESTER (Japan) is used to measure A.C. Electrical Conductivity at the University of Babylon/College of Education for Pure Sciences/Physics Department figure (3.5) shows a diagram for the A.C electrical measurement system. Only (1cm) from each one of the samples has been taken and put between two electrodes and by different frequencies from (100Hz-5MHz) at room temperature. The capacity and dissipated factor have been recorded for all 5 the samples. Dielectric constant, dielectric loss and conductivity have been calculated from this data.

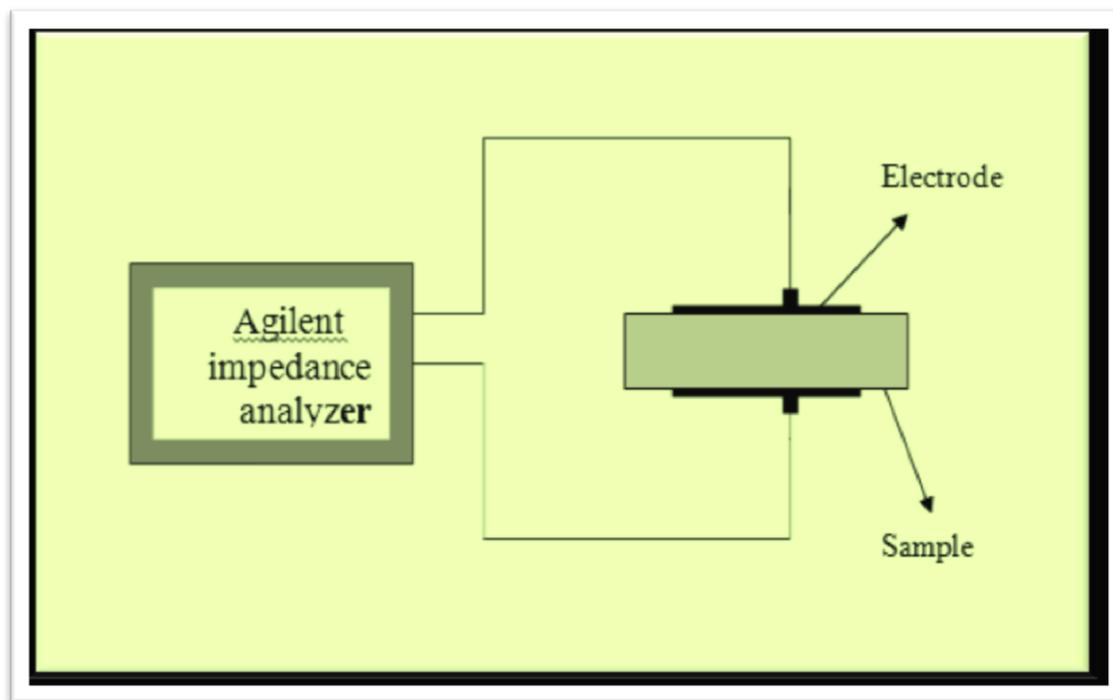
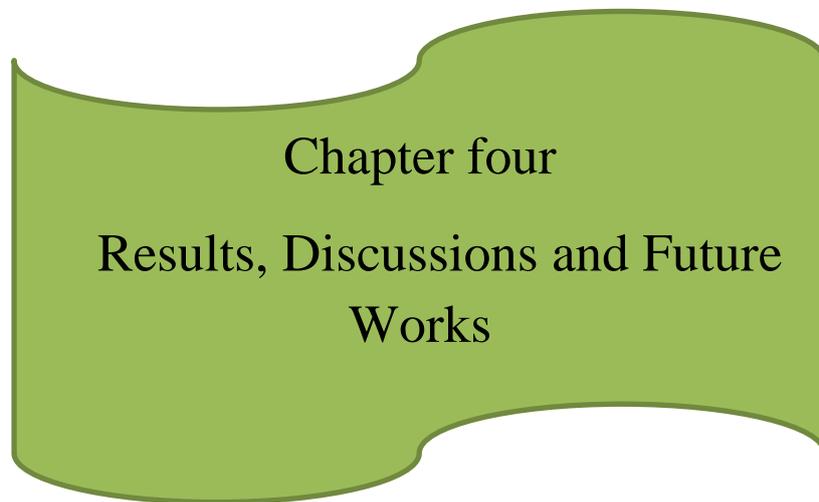


Figure (3.5): Diagram for system of A.C electrical measurement system

3.7 Application of (PVA-BaTiO₃-TiO₂) Nanocomposite Films

Antimicrobial activity of the (PVA-BaTiO₃-TiO₂) nanocomposites tested samples were determined using a disc diffusion method. The antibacterial activities were done by using gram positive organisms (*Staphylococcus aureus*) and gram negative organisms, *Escherichia coli*, Bacteria (*Staphylococcus aureus* and *Escherichia (coli)*) were cultured in Muller-Hinton agar. The disks of the (PVA-BaTiO₃-TiO₂) nanocomposites were placed over the media and incubated at 37°C for 24 hours. The inhibition zone diameter was measured.



Chapter four
Results, Discussions and Future
Works

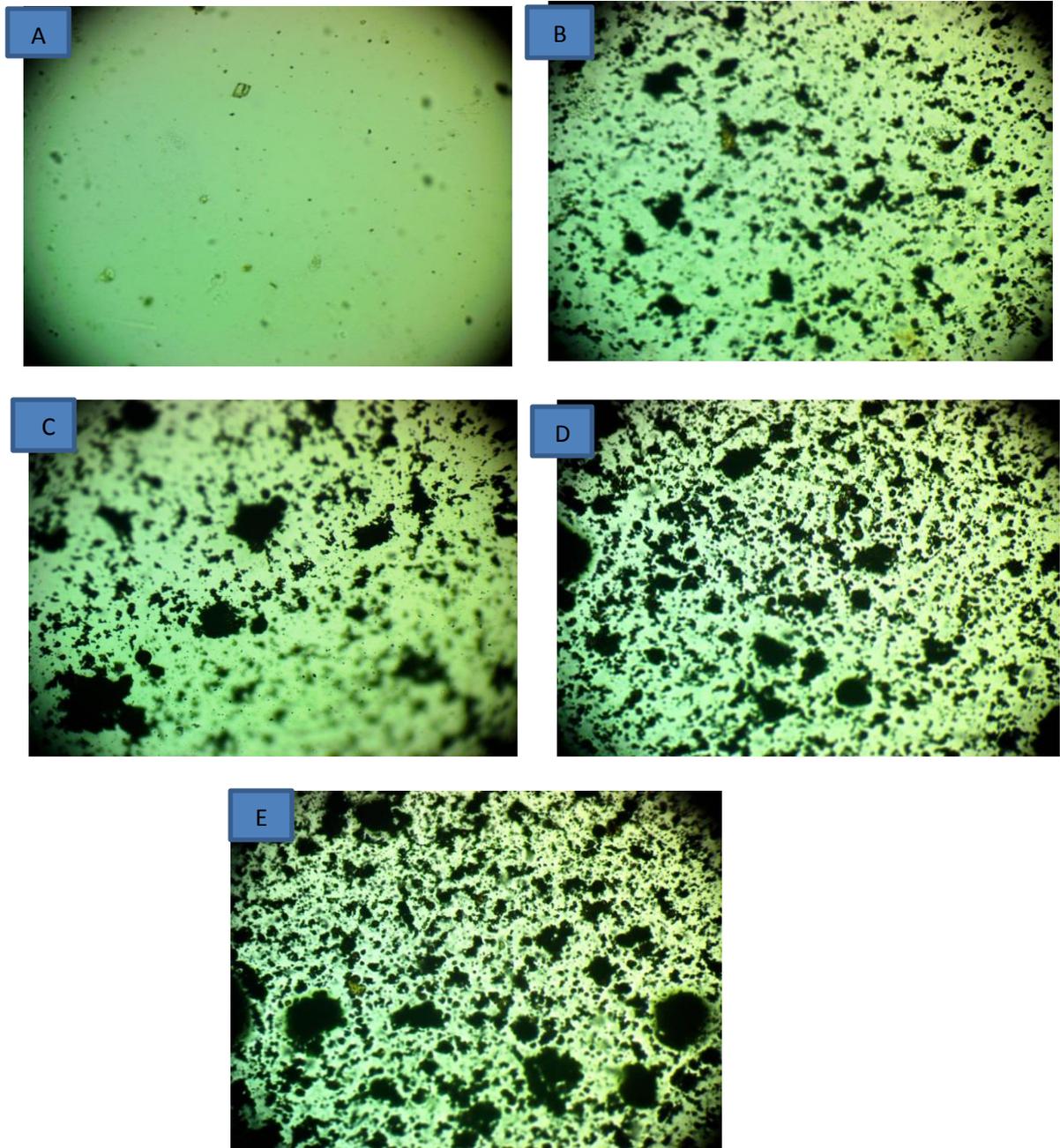
4.1 Introduction

This chapter includes the findings as well as a review of the systemic, optical and (A.C) electrical and application measurements for (PVA-BaTiO₃-TiO₂) nanocomposites. It will also discuss the effect of different concentrations additive nanoparticles (BaTiO₃ and TiO₂) in the optical microscope, Fourier transform infrared ray (FTIR), scanning electron microscope (SEM)

4.2 The Structural Properties.

4.2.1 The Optical Microscope

Images of (PVA-BaTiO₃-TiO₂) nanocomposites films taken at a magnification power of 10x for samples of various concentrations are shown in figure (4.1). As shown in figure (4.1)(A, B, C, D, E). when the concentration of BaTiO₃ and TiO₂ reach 2.5 wt.% the nanoparticles form a continuous network in films (Polyvinyl alcohol), inside the polymers, the nanoparticles are linked in this network includes routes for charge carriers to travel through, causing a shift in the material properties. [97].



Figure(4.1). The photomicrographs(10)x for (PVA-BaTiO₃-TiO₂) Nanocomposites : (A) For pure (PVA), (B) For1wt% (C) For 1.5wt%, (D) For 2 wt% ,(E) For 2.5wt%.

4.2.2 Fourier Transform Infrared Ray(FTIR)

FTIR spectroscopy has been used to investigate interactions between atoms or ions in the (PVA-BaTiO₃-TiO₂) nanocomposites, these interactions take in changes in the nanocomposites' vibrational methods are shown in figure (4.2) (A, B, C, D, and E). The stretching vibration of a hydroxyl group (OH) of PVA is given a bandwidth of around 3300 cm⁻¹ in this FTIR spectrum for (PVA) films, which may be related to the polymer and nanoparticles' intermolecular type of hydrogen bonding. At around 2930 cm⁻¹, the band corresponding to CH₂ asymmetric stretching vibration occurs. This C=O, C=C stretching kind is responsible for the peaks at 1710 and 1652 cm⁻¹. The wagging (CH) group has been assigned the absorption peak at 1240 cm⁻¹. The 1105 cm⁻¹ band relates to the C-O stretching of carbonyl sets on this PVA backbone. While out of plane rings C-H bending is given an absorption band of roughly 1963cm⁻¹. The interaction of the polymer with BaTiO₃ and TiO₂ causes a transition in the (PVA) spectrum. This is owing to the fact that there are no interactions between the (PVA) and (BaTiO₃ - TiO₂) nanoparticles. According to FTIR analyses, the transmittance is lowered due to a minor increase in BaTiO₃ and TiO₂ concentrations [98]. as shown in the table (4.1).

Table (4.1): FTIR Transmittance bands positions and their assignments for pure (PVA).

Wavenumber (cm ⁻¹)	Band assignment
3300	OH stretching
2930	CH ₂ asymmetric stretching
1652	C=C stretching
1710	C=O stretching
1429	Symmetric bending of CH ₂
1326	(CH+OH) bending
1241	Wagging of (CH)
1105	C-O stretching
963	Out of plane rings C-H bending
845	CC stretching Vibrations
663	Wagging mode of (OH) groups
481	Bending mode of (CO)
421	Wagging of (CO)

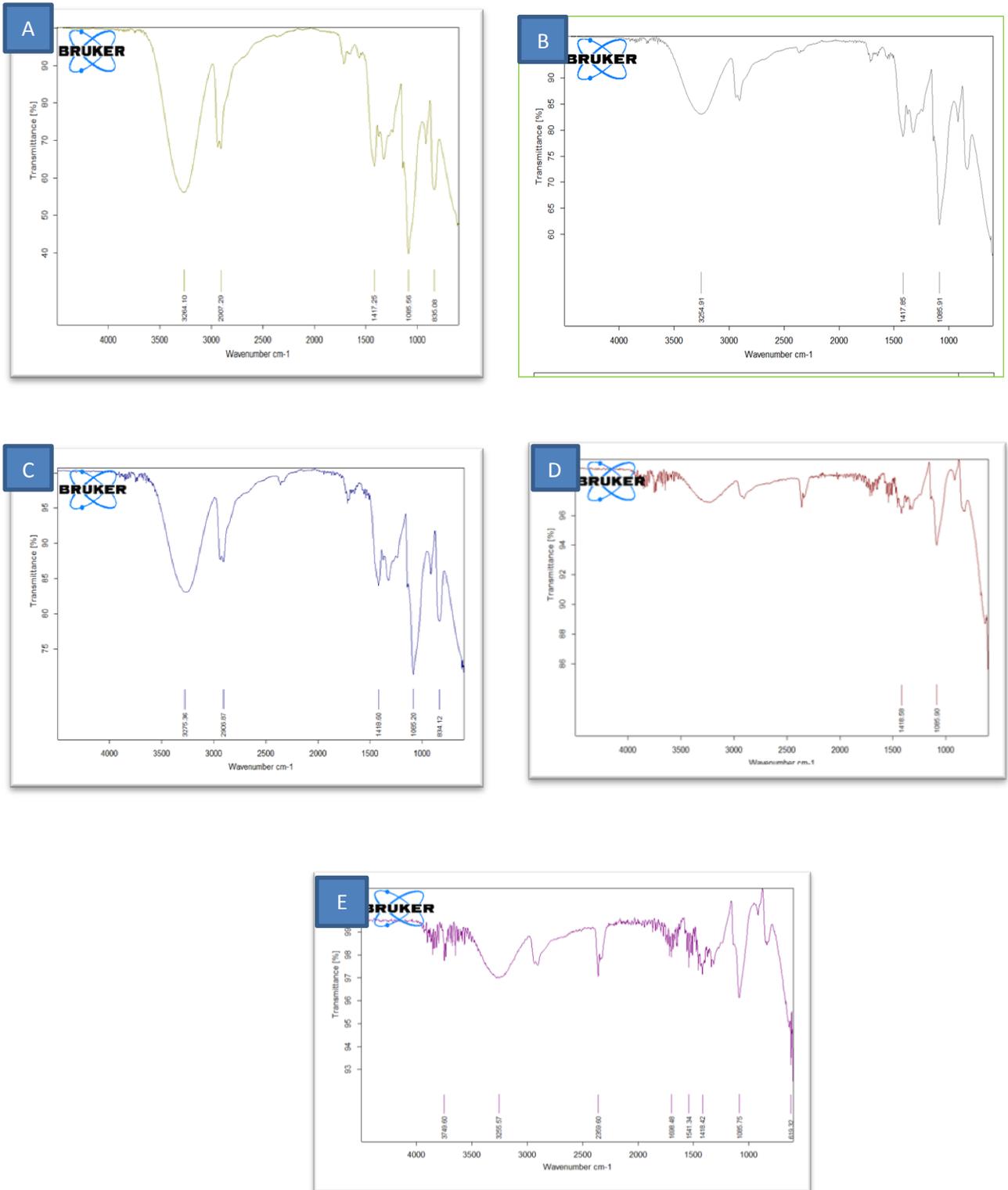


Figure (4.2). FTIR spectra For (PVA-BaTiO₃-TiO₂) Nanocomposites: (A) For (PVA), (B) For 1wt% (C) For 1.5wt%, (D) For 2 wt% , (E) For 2.5wt%.

4.2.3 Scanning Electron Microscopy (SEM)

SEM is used to analyze the dispersion of nanocomposites particles in the polymer matrix and to thoroughly investigate the effect of barium titanate and titanium dioxide nanoparticles material. Figure (4.3) shows typical SEM images of (PVA-BaTiO₃-TiO₂) nanocomposites films and with different concentrations of barium titanate and titanium dioxide nanoparticles material. It was found to be smoother, more homogeneous, and more coherent in image (A) in figure (4.3). Though gradually growing the nanoparticles ratio in polymer (B, C, D, E), surface morphology shifts. The appearance of several spherical particle aggregates or chunks on the surface of the nanocomposites films indicates the presence of a homogeneous growth mechanism. It gets softer as the concentration of both nanoparticles increases. the (BaTiO₃ –TiO₂) nanoparticles aggregate and are well distributed in (PVA-BaTiO₃-TiO₂) nanocomposites films (4.3-B, C, D, and E). When (BaTiO₃ –TiO₂) nanoparticles are added to(PVA) composites at a concentration of 2.5%, they form a continuous within the network polymer [99].

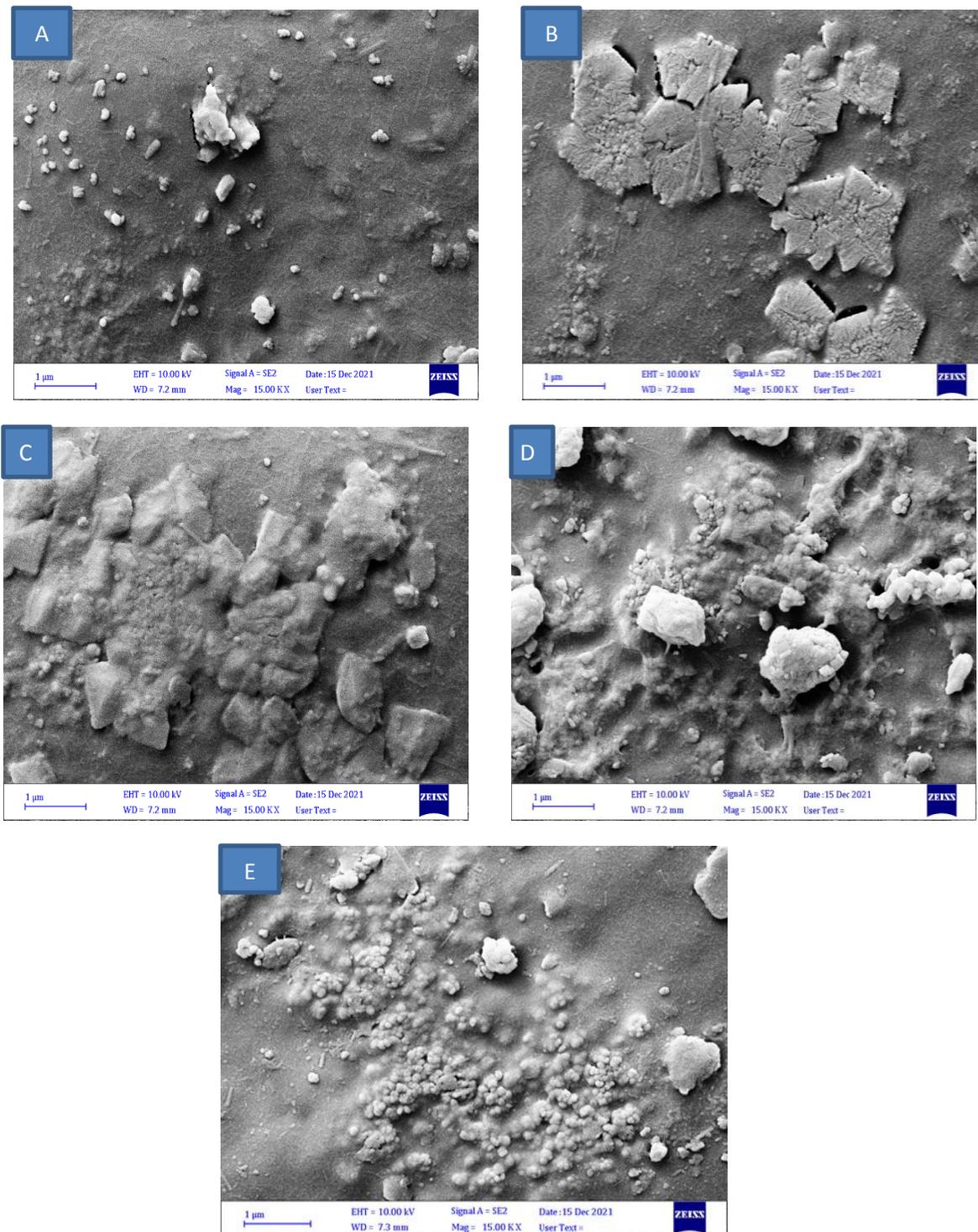


Figure (4.3). The Photomicrographs For (PVA-BaTiO₃-TiO₂) Nanocomposites: (A) For (PVA), (B) For 1wt% (C) For 1.5wt%, (D) For 2 wt%, (E) For 2.5wt%

4.3 The Optical Properties

The main purpose of studying the optical properties of the (PVA-BaTiO₃-TiO₂) nanocomposites is to identify the effect of adding the barium titanate and titanium dioxide nanoparticles on the optical properties. The research involves measuring the absorbance spectrum of (PVA-BaTiO₃-TiO₂) films at room temperature, and determining the absorbance, extinction, and other optical constants, defining the forms of electronic transitions, and measuring energy gaps.

4.3.1 Absorbance (A)

Figure (4.4) shows relationship between absorbance and wavelength of (PVA-BaTiO₃-TiO₂) nanocomposite. It can be noticed from the figure that the absorbance for all films has a high value at a wavelength in the neighborhood of the fundamental absorption edge (220 nm), then the absorbance decreases with the increase of wavelength. In general, the absorbance of films has low values in the visible and near- infrared regions. This behavior can be explained as follows: When the wavelength decreases (near the fundamental absorption edge), the incident photon interacts with the material, and absorbance increases [100]. In other words, the incident light absorbs by the free electrons. Consequently, by the increase of the weight percentages of BaTiO₃ and TiO₂ nanoparticles absorbance is increased transmitted. In other words, the incident light absorbs by the free electrons. Consequently, by the increase of the weight percentages of BaTiO₃ and TiO₂ nanoparticles absorbance is increased.

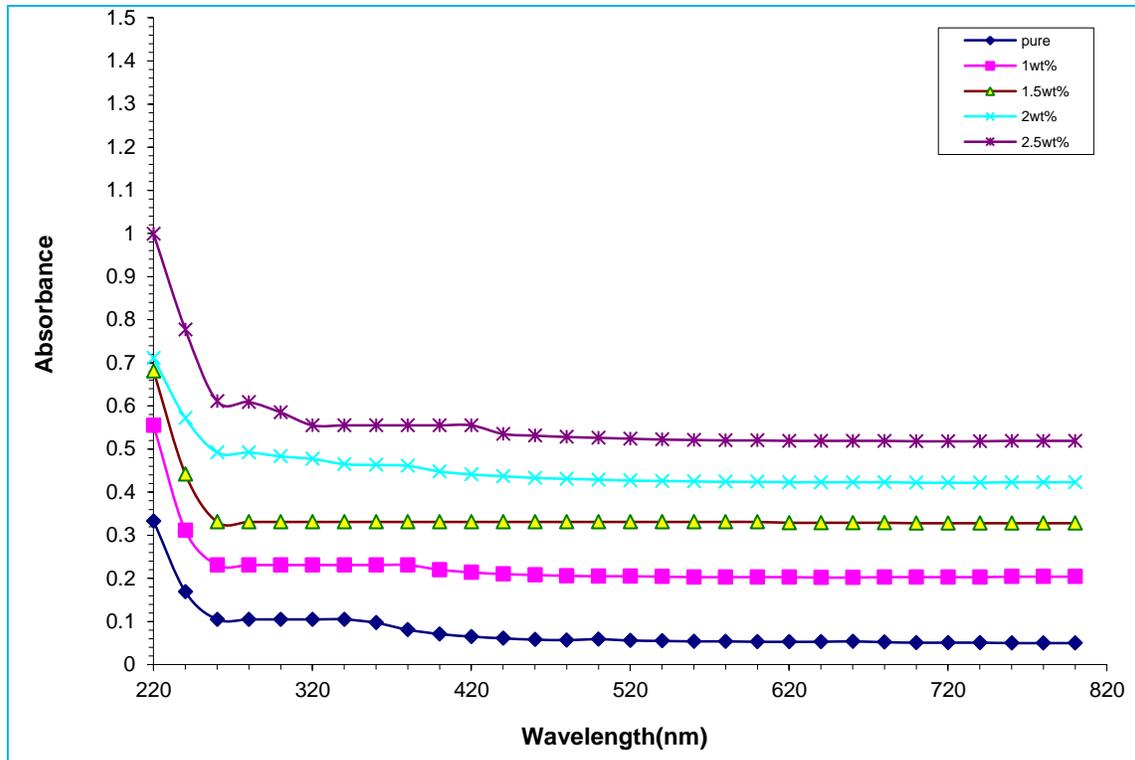


Figure (4.4) Relationship between absorbance and wavelength of (PVA-BaTiO₃- TiO₂) nanocomposites.

4.3.2 Transmittance Spectrum

Figure (4.5) shows relationship between transmittance and wavelength of (PVA-BaTiO₃-TiO₂) nanocomposites, from this figure that transmittance decrease with the increased concentration of (BaTiO₃-TiO₂) nanoparticles, this is caused by added (BaTiO₃-TiO₂) nanoparticles contain electrons in it are outer orbits can absorb the electromagnetic energy of the incident light and travel to higher energy levels, this process is not accompanied by the emission of radiation because the traveled electron to higher levels has occupied vacant positions of energy bands, thus part of the incident light is absorbed by the substance and does not penetrate through it, on the other hand, the pure (PVA) has high transmittance because there are no free electrons (i.e. electrons are linked to atoms by covalent bonds), this is

because the breaking of electron linkage and moving it to the conduction band need to photon with high energy [101].

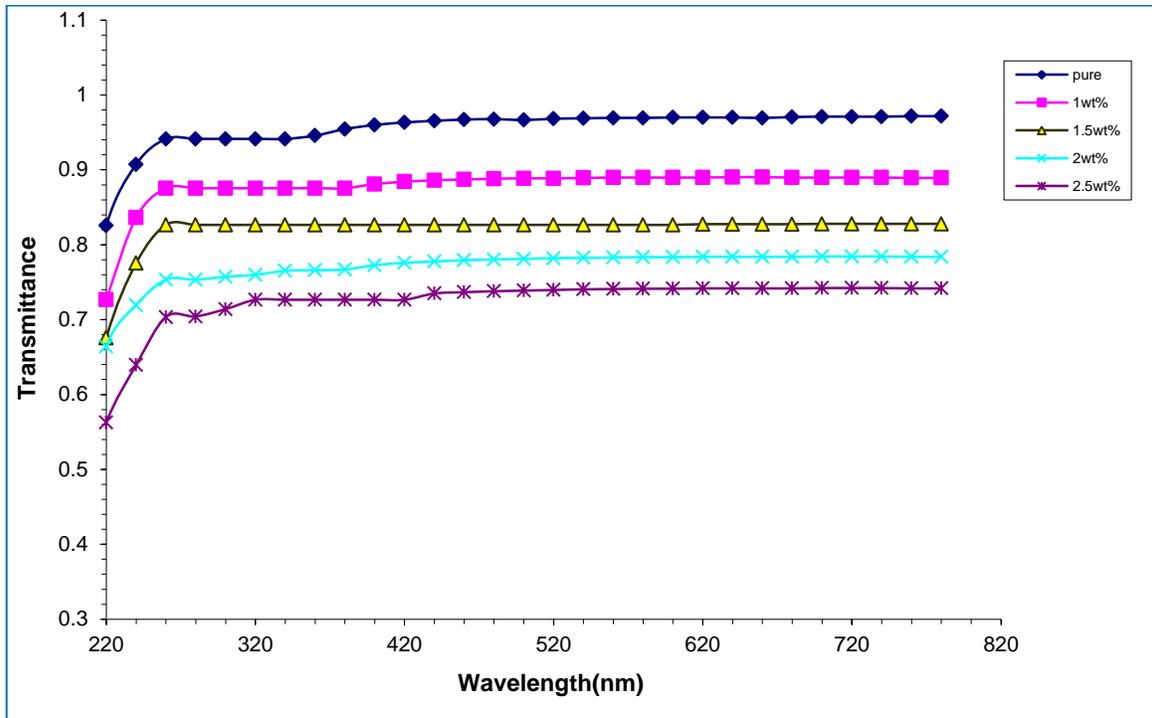


Figure (4.5) Relationship between transmittance and wavelength of (PVA-BaTiO₃-TiO₂) nanocomposites.

4.3.3 Absorption Coefficient (α) of (PVA-BaTiO₃-TiO₂) nanocomposites

Figure (4.6) show the relationship between absorption coefficient and photon energy for (PVA-BaTiO₃-TiO₂) nanocomposites. The absorption coefficient α is calculated by using equation (2.7). It can be seen that the absorption coefficient is the smallest at high wavelength and low energy, this means that the possibility of electron transition is little because the energy of the incident photon is not sufficient to move the electron from the valence band to the conductive band ($h\nu < E_g$) [102]. At high energies absorption is bigger, this indicates that there is a high likelihood of electron transitions. As a result, the incident photon's energy is sufficient to transfer the electron from the valence band to the conduction band,

indicating that the incident photon's energy exceeds the forbidden energy difference. This demonstrates how the absorption coefficient can help determine the nature of an electron transfer, when the values of the absorption coefficient are high ($\alpha > 10^4$) cm^{-1} at high energies it is expected that direct transition of an electron occurs, the energy and moment are maintained by the electrons and photons, on the other hand, because the values of the absorption coefficient are low ($\alpha < 10^4$) cm^{-1} at low energies, it is expected that indirect transition of an electron occurs, and the electronic momentum is maintained with the assistance of the phonon [103]. among other results is that the coefficient of absorption for the (PVA-BaTiO₃-TiO₂) nanocomposites is less than (10^4 cm^{-1}), this explain that the electron transition is indirect.

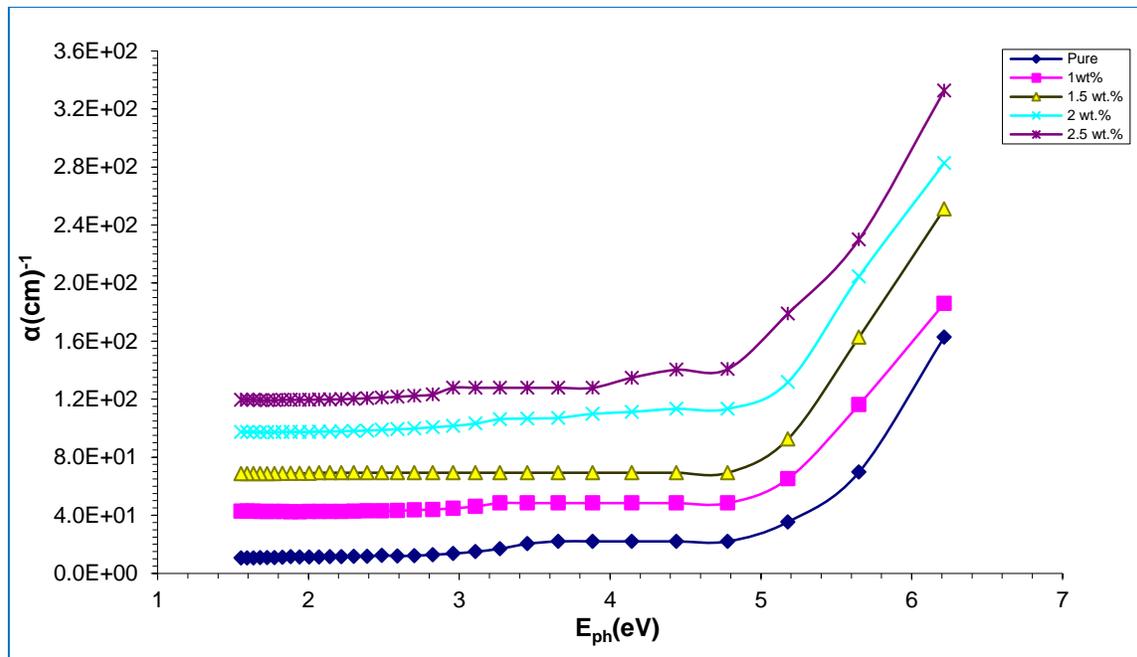


Figure (4.6) Relationship between absorption coefficient and photon energy of (PVA-BaTiO₃-TiO₂) nanocomposites.

4.3.4 Optical Energy Gaps of the (Allowed and Forbidden) Indirect Transition

Both the allowed and forbidden indirect transition band energy gap has been

calculated using equation (2.4). figure (4.7) shows the relation between absorption edge $(\alpha h\nu)^{1/2}$ and photon energy of (PVA-BaTiO₃-TiO₂) nanocomposites and the photon energy, on drawing a straight line from the upper part of the curve toward the (x) axis at the value $(\alpha h\nu)^{1/2} = 0$ we get the energy gap for the allowed indirect transition. The obtained values are shown in table (4.3). The values of the energy gap decrease with increasing weight percentages of barium titanate and titanium dioxide nanoparticles. This attributed to the creation of localized levels in the forbidden energy gap [104], The transfer, in this case, occurs in two steps, with an electron moving from the valence band to the local levels and then to the conduction band as the weight percentage of barium titanate and titanium dioxide nanoparticles increases. This behavior is due to the heterogeneous nature of nanocomposites (i.e. the electronic conduction depends on added concentration), the density of the localized state increased with increasing of the concentration of (BaTiO₃-TiO₂) nanoparticles [104].

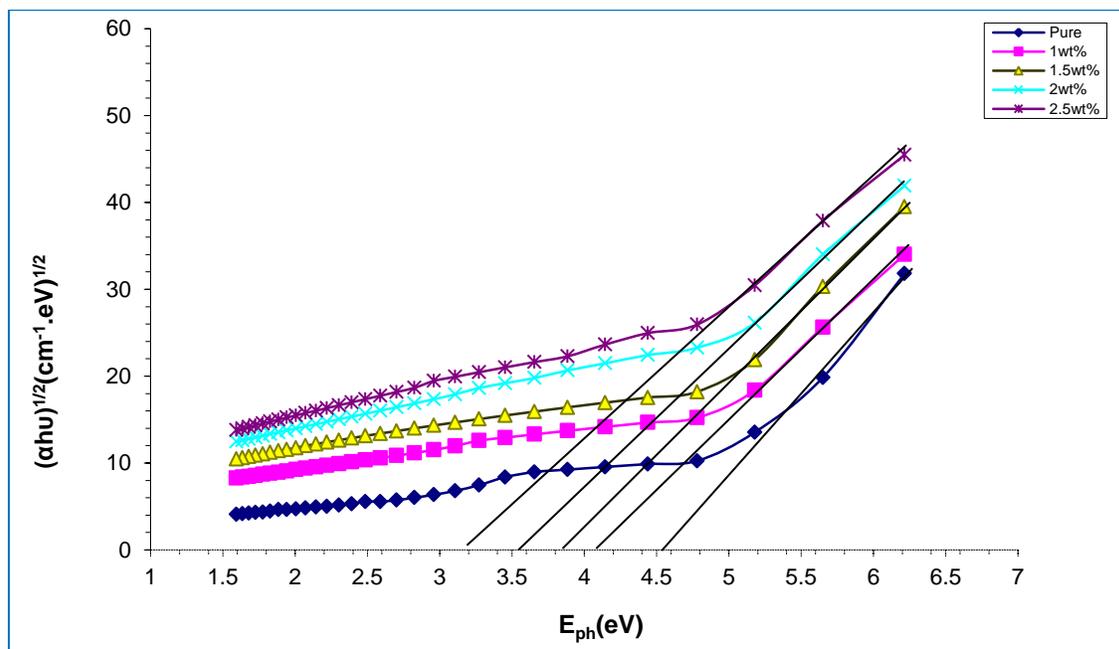


figure (4.7) Relationship between absorption edge $(\alpha h\nu)^{1/2}(\text{cm}^{-1}.\text{ev})^{1/2}$ and photon energy of (PVA-BaTiO₃-TiO₂) nanocomposites.

The forbidden transition of the indirect energy gap is calculated in the same way.

Figure (4.8) shows the forbidden transition of the indirect energy gap for the (PVA-BaTiO₃-TiO₂) nanocomposites

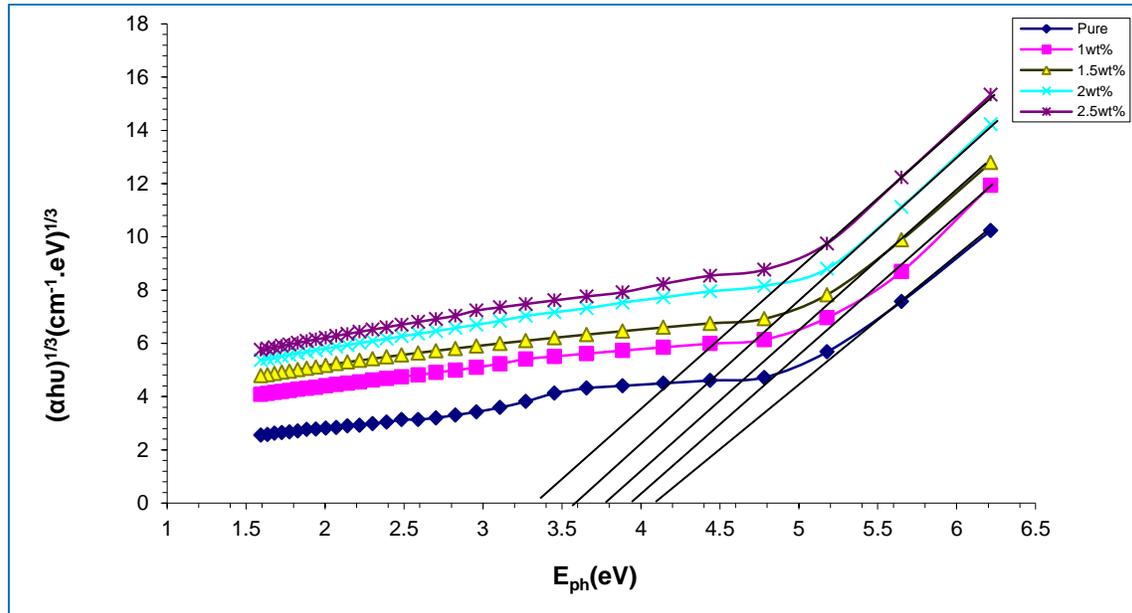


Figure (4.8) Relationship between $(ahv)^{1/3}$ ($\text{cm}^{-1}\cdot\text{eV}$)^{1/3} and photon energy of (PVA-BaTiO₃-TiO₂) nanocomposites.

Table (4.1): The values of energy gap for the allowed and forbidden indirect transition for(PVA-BaTiO₃-TiO₂) nanocomposites.

Barium titanate and Titanium dioxide nanoparticles wt. %	The values of the optical energy gap for the indirect transition (eV)	
	Allowed	forbidden
0	4.5	4.3
1	4.1	4
1.5	3.9	3.7
2	3.5	3.5
2.5	3.4	3.3

4.3.5 Refractive Index (n)

The refractive index (n) is calculated from equation (2.11). Figure (4.9) shows relationship between refractive index and wavelength of (PVA-BaTiO₃-TiO₂) nanocomposites. It is obvious from the figure that the refractive index increase with increasing weight percentages of the concentration of (BaTiO₃-TiO₂) nanoparticles to the (PVA) because of increasing in density nanocomposites. In the ultraviolet region, high refractive index values are observed due to the low transmittance in this region, while in the visible region, low values are observed due to the high transmittance in this region [105].

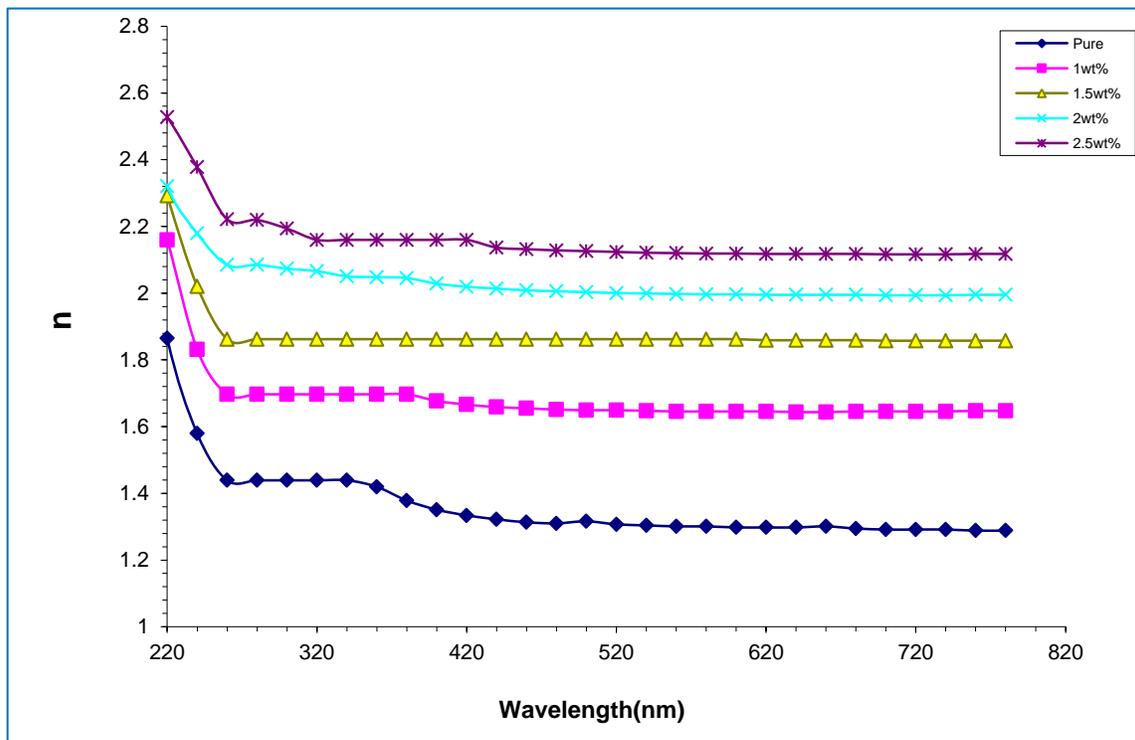


Figure (4.9). Relationship between refractive index and wavelength of (PVA-BaTiO₃-TiO₂) nanocomposites.

4.3.6 Extinction Coefficient (k)

The extinction coefficient (k) is calculated by using equation (2.12). Figure (4.10) shows relationship between extinction coefficient and wavelength of (PVA- BaTiO_3 - TiO_2) nanocomposite. It can be noted that the extinction coefficient increases with the increase of (BaTiO_3 - TiO_2) nanoparticles. This is attributed to the increased absorption coefficient with the increase of weight percentages of Barium titanate and Titanium dioxide nanoparticles. This result indicates that the atoms of (BaTiO_3 - TiO_2) nanoparticles will modify the structure of the host polymer [106].

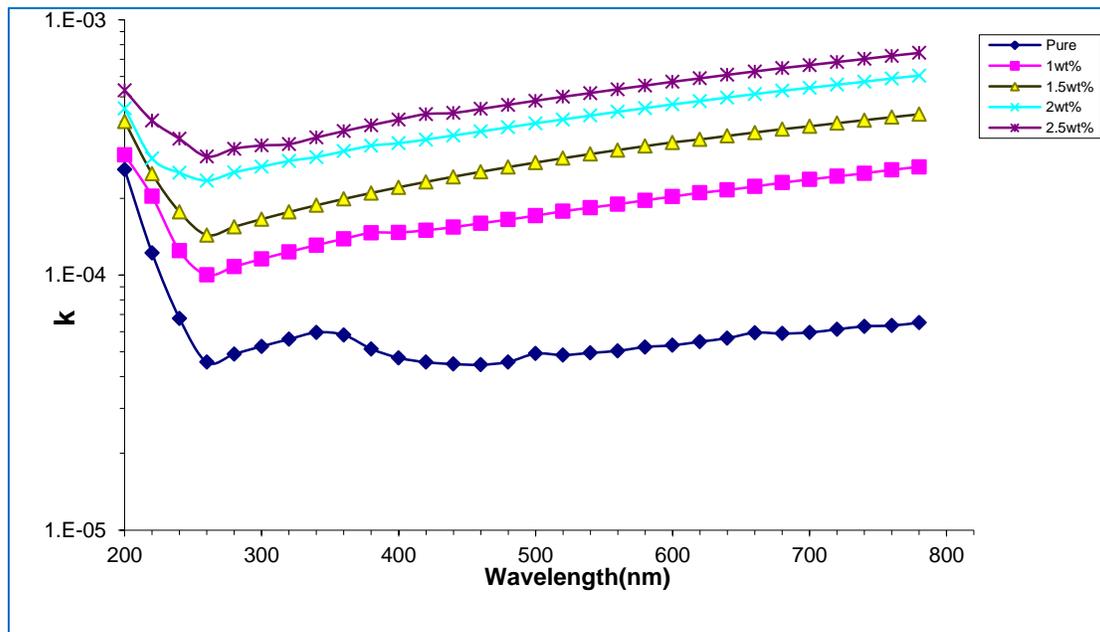


Figure (4.10) Relationship between extinction coefficient and wavelength of (PVA- BaTiO_3 - TiO_2) nanocomposites.

4.3.7 Real and Imaginary Parts of Dielectric Constant (ϵ_1 , ϵ_2)

The dielectric constant for two parts (real and imaginary) for (PVA- BaTiO_3 - TiO_2) nanocomposites have been calculated from equations (2.16) and (2.17),

respectively. Figure(4.11) shows the relationship between real part of dielectric constant and wavelength of (PVA-BaTiO₃-TiO₂) nanocomposites. It can be seen from the figure that (ϵ_1) considerably dependent on (n^2) due to the low value of (k^2) also, the real dielectric constant is increased with the increase of the concentrations of (BaTiO₃-TiO₂) nanoparticles[107]. Figure (4.12) shows relationship between imaginary part of dielectric constant and wavelength of (PVA-BaTiO₃-TiO₂) nanocomposites. It can be seen from the figure that (ϵ_2) is dependent on (k) values that are changing with the change of the absorption coefficient due to the relation between (α) and (k) [107].

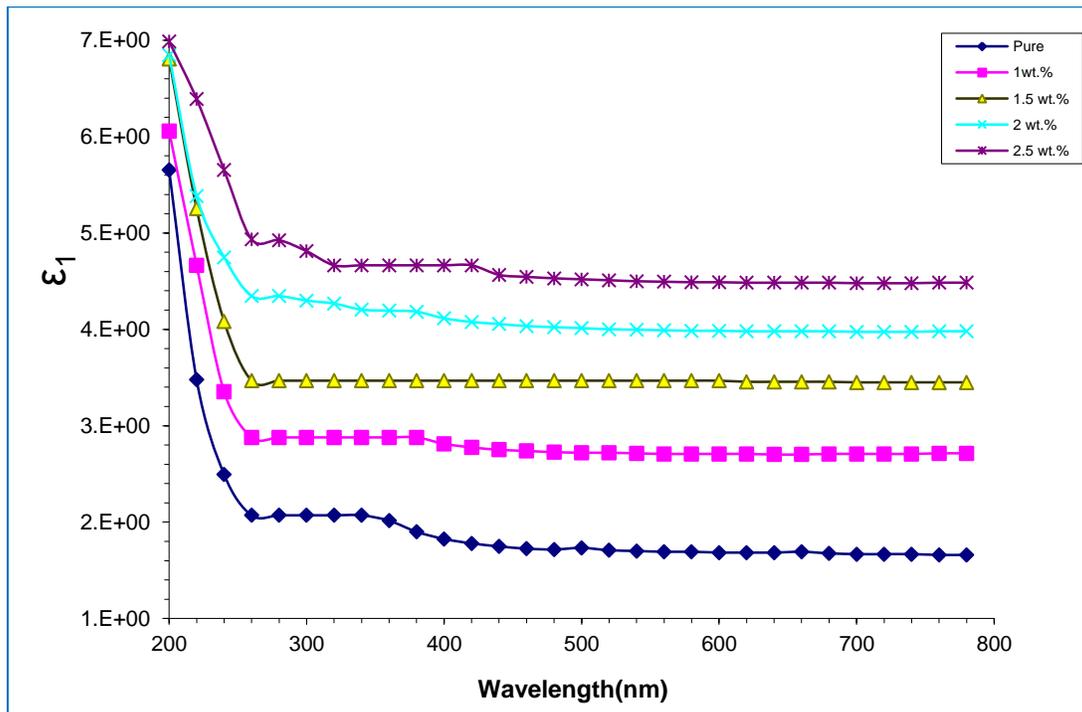


Figure (4.11) Relationship between real part of dielectric constant and wavelength of (PVA-BaTiO₃-TiO₂) nanocomposites.

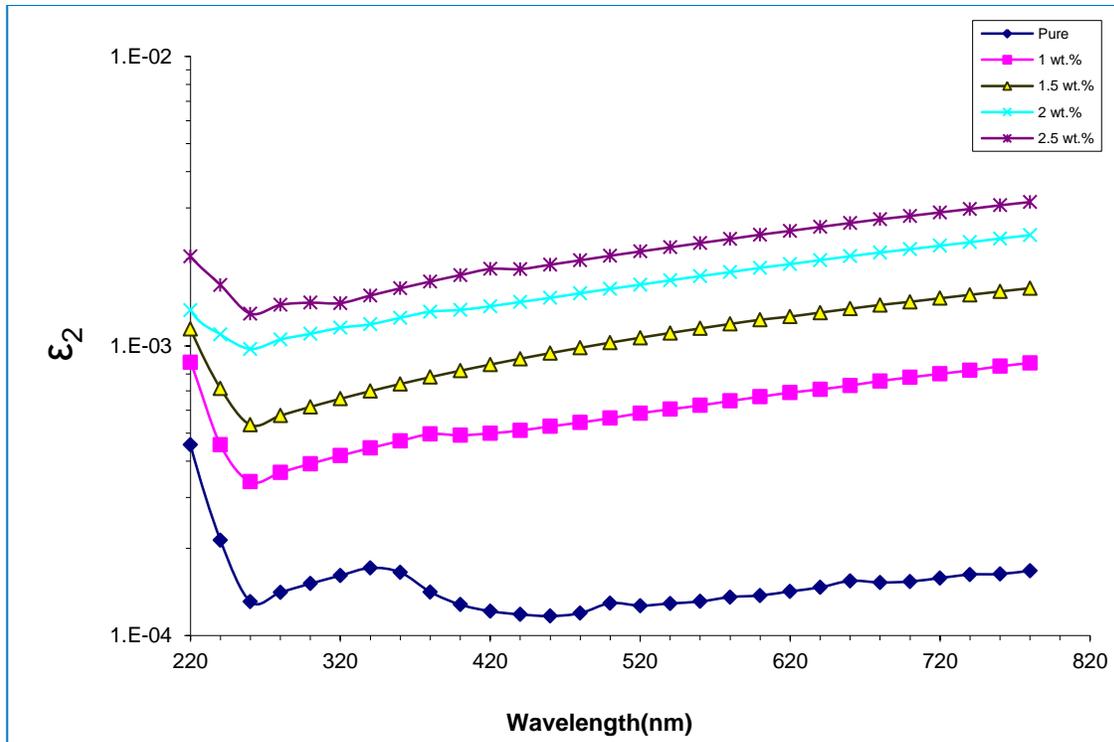


Figure (4.12) Relationship between imaginary part of dielectric constant and wavelength of (PVA-BaTiO₃-TiO₂) nanocomposites.

4.3.8 Optical Conductivity (σ_{op})

The optical conductivity is calculated using equation (2.18). Figure (4.13) shows the relationship between optical conductivity and wavelength of (PVA-BaTiO₃-TiO₂) nanocomposites. It was observed that the optical conductivity increases as the percentages of (BaTiO₃-TiO₂) in the (PVA) increase to (2.5 wt.%). This increase due to the creation of new levels in the band gap leads to facilitate the crossing of electrons from the valence band to these local levels to the conduction band, consequently the band gap decreases, and the conductivity increases [108].

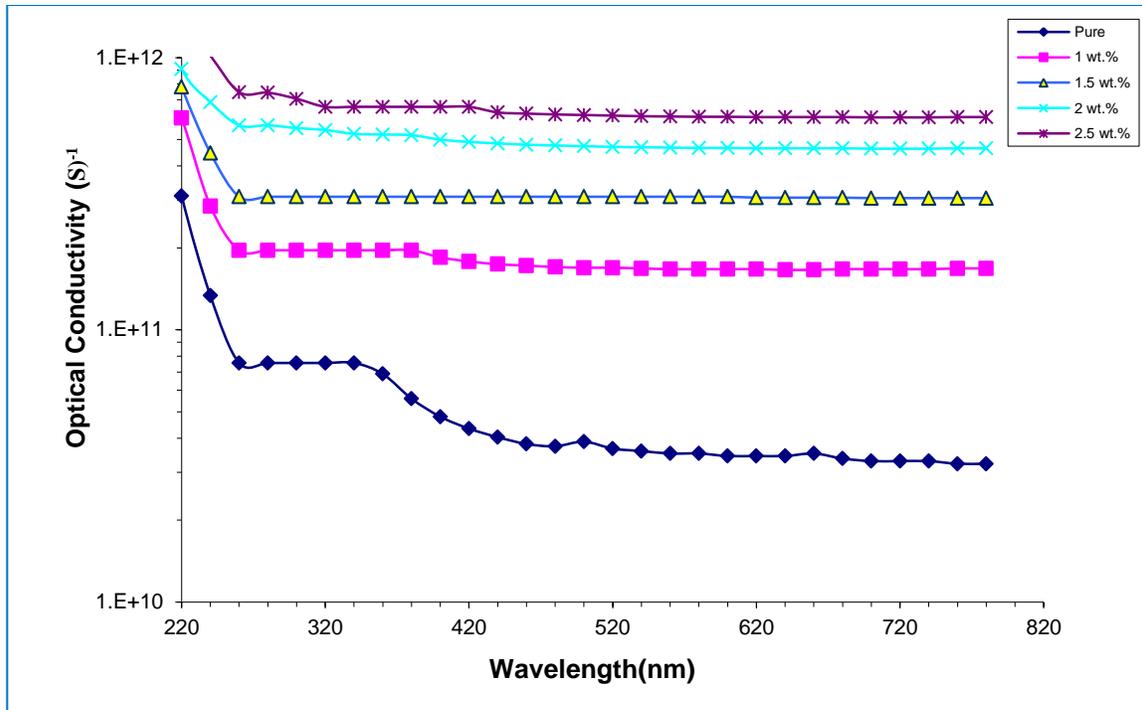


Figure (4.13) Relationship between optical conductivity and wavelength of (PVA-BaTiO₃-TiO₂) nanocomposites.

4.4 - The A.C Electrical Properties of (PVA-BaTiO₃-TiO₂) Nanocomposites

The A.C electrical properties for the (PVA-BaTiO₃-TiO₂) nanocomposites were studied within frequency ranging from (100Hz -5MHz) at room temperature. The dielectric constant, which is the most important of A.C properties were calculated using the equation (2.41). The dielectric loss was calculated by equation (2.35), using the measured dielectric constant and ($\tan \delta$), while the A.C electrical conductivity σ A.C was calculated by equation (2.42) after substituting the measured values of (ϵ').

4.4.1 - The Dielectric Constant for (PVA-BaTiO₃-TiO₂) Nanocomposites

Figure (4.14) shows the relationship between dielectric constant and concentration of (BaTiO₃-TiO₂) nanoparticles. It can see the dielectric constant increases with

the increase of the weight percentages of barium titanate and titanium dioxide. The reason for this increase in the values of the dielectric constant is an increase in the carriers of charge and also the formation of a continuous network of $(\text{BaTiO}_3 - \text{TiO}_2)$ ions inside the composite [109]. This was well shown in the microscopic photos taken for samples of $(\text{PVA}-\text{BaTiO}_3-\text{TiO}_2)$ nanocomposites at different concentrations. At low concentration (1wt.%) of the barium titanate and titanium dioxide nanoparticles take the form of cluster or separated groups; hence, the dielectric constant becomes approximately low. On the other hand, at high concentrations (2.5wt.%), barium titanate and titanium dioxide nanoparticles form a continuous network within the nanocomposites, so the dielectric constant rises in proportion to the volumetric rate of the barium titanate and titanium dioxide nanoparticles [109].

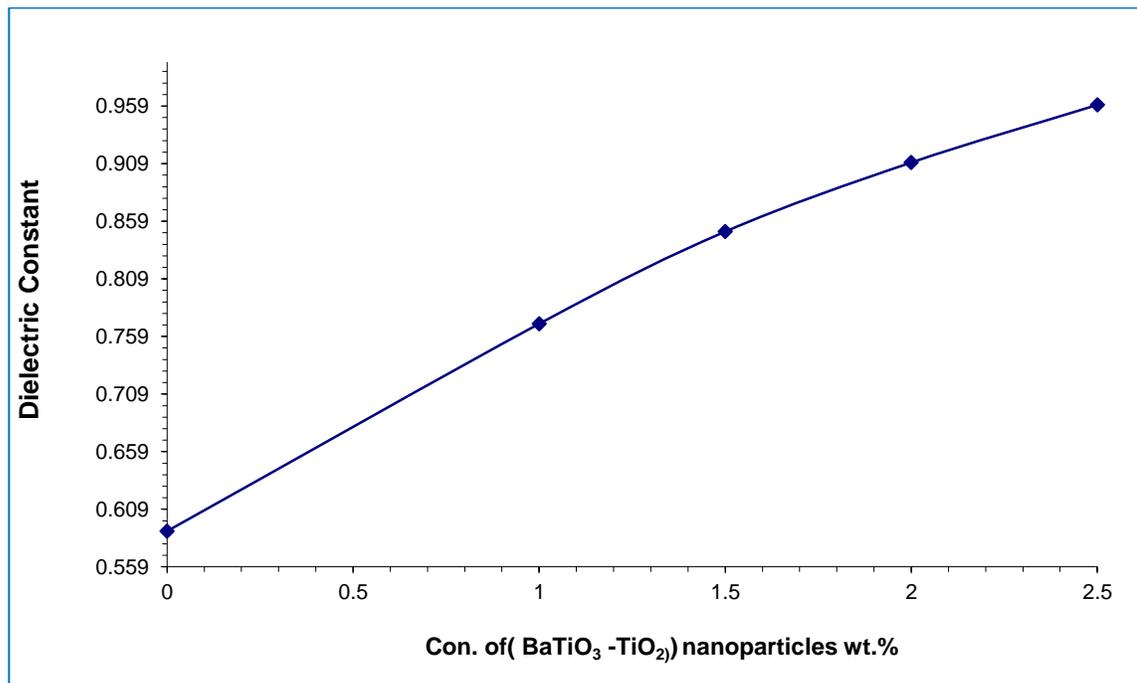


Figure (4.14) Relationship between dielectric constant and concentration of $(\text{BaTiO}_3-\text{TiO}_2)$ nanoparticles.

Figure (4.15) shows the relationship between dielectric constant and frequency for (PVA-BaTiO₃-TiO₂) nanocomposites. The figure shows that the dielectric constant values decrease with increasing applied frequency, the increase of frequencies result in decreasing of space charge polarization to the total polarization. The space charge polarization becomes the more contributing type of polarization at low frequencies, and less contributing with the increase of frequency; this would result in the decrease of dielectric constant values for all samples of (PVA-BaTiO₃-TiO₂) nanocomposites with the increase of the electric field frequency [110]. The other types of polarizations appear at subsequent frequencies, the ionic polarization reacts slightly to the variation in the field frequencies compared with electronic polarization, this is due to the mass of an ion is greater than that of the electron. The electrons respond to even the high frequencies of the field vibrations. Electronic polarization was the only form of polarization available at higher frequencies due to the low mass of electrons. At high frequencies, the dielectric constant becomes nearly constant [110].

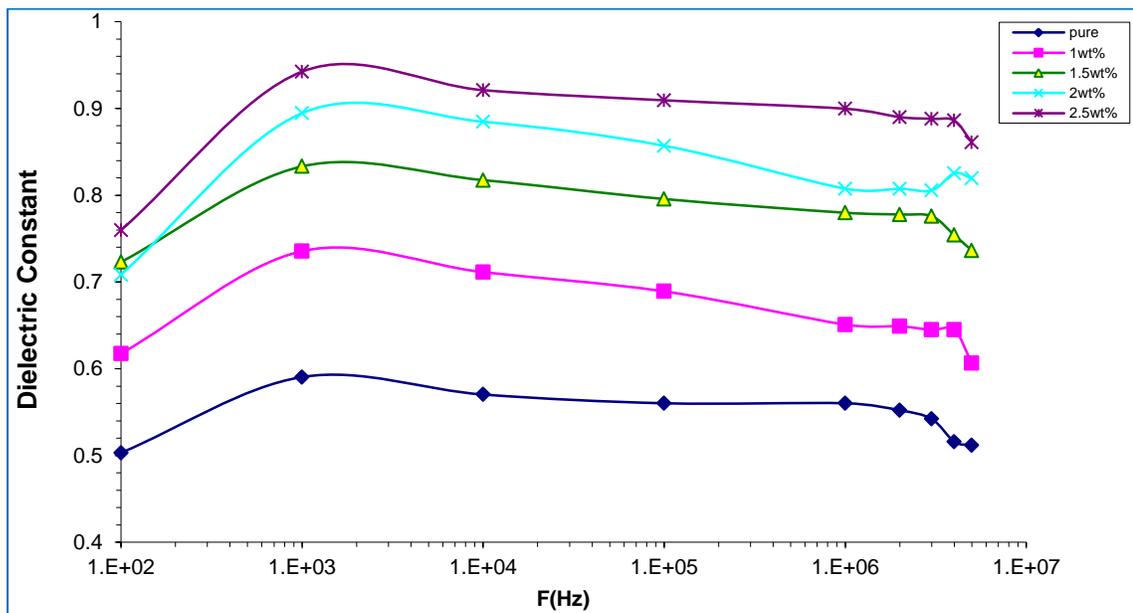


Figure (4.15) Relationship between dielectric constant and frequency for (PVA-BaTiO₃-TiO₂) nanocomposites.

4.4.2- The Dielectric Loss of (PVA-BaTiO₃-TiO₂) Nanocomposites

Figure (4.16) shows the relationship between dielectric loss and concentration of (BaTiO₃-TiO₂) nanoparticles. It is obvious from the figure that the values of dielectric loss are increasing by increasing the concentration of (BaTiO₃-TiO₂) nanoparticles due to the increase of the charge carriers caused by the increase of (BaTiO₃-TiO₂) nanoparticle concentration [111]. Figure (4.17) shows the relationship between dielectric loss and frequency of (PVA-BaTiO₃-TiO₂) nanocomposite. It is obvious from the figure that the values of dielectric loss, are high at low applied frequency but they decrease with increasing frequency. This attributed to the decrease of the space charge polarization contribution when increasing the frequency. The highest value of the dielectric loss at $f=1$ KHz for (PVA-BaTiO₃-TiO₂) nanocomposites, this value represents the highest dielectric loss at a certain frequency, that is the highest absorption of an applied field. The absorption happens due to the Maxwell-Wagner phenomenon which is caused by A.C current due to the difference of dielectric constant and conductivity of the phases in the nanocomposites [111]. When the frequency is increasing to 2MHz, the dielectric loss is approximately constant for (PVA-BaTiO₃-TiO₂) nanocomposites. This is attributed to the mechanism of other types of polarization that occurs at high frequencies [111].

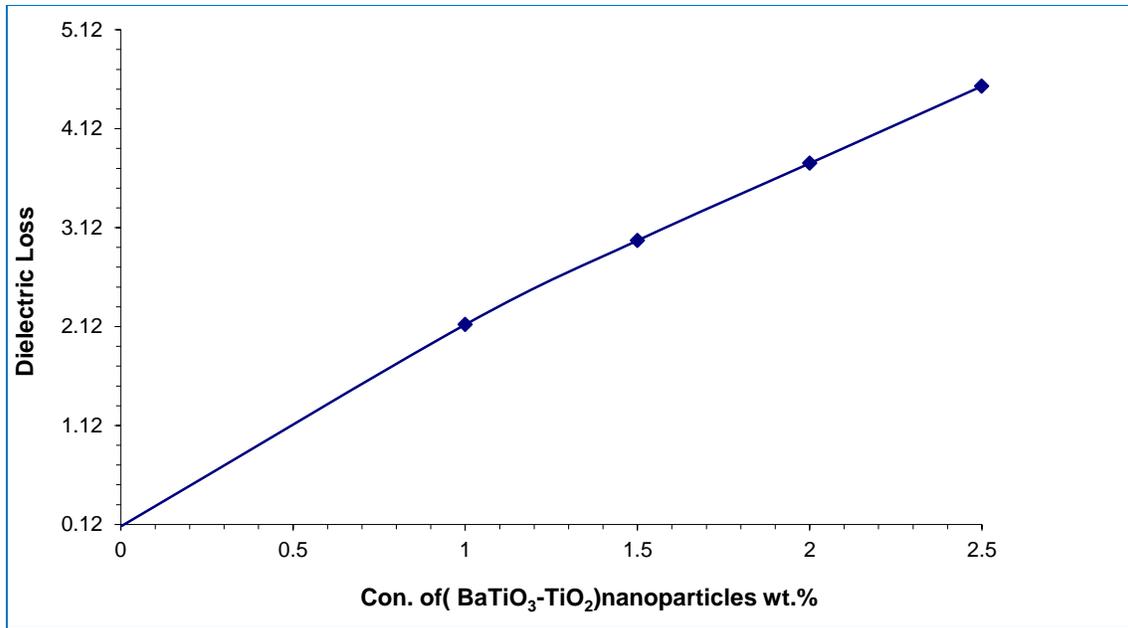


Figure (4.16) Relationship between dielectric loss and concentration of (BaTiO₃-TiO₂) nanoparticles.

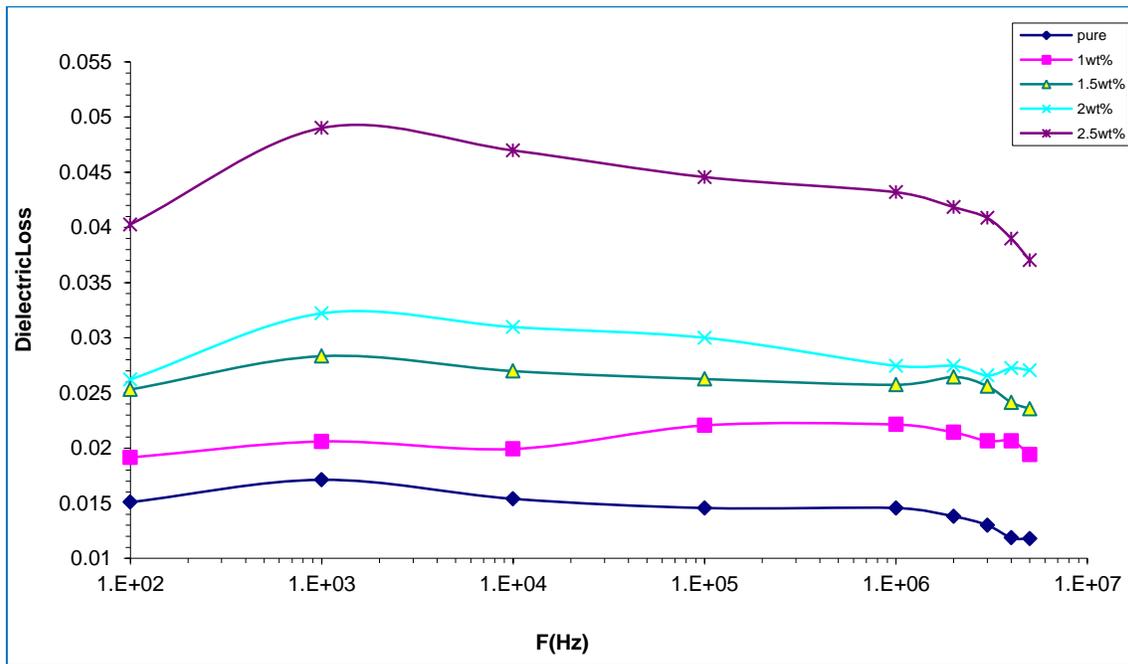


Figure (4.17) Relationship between dielectric loss and frequency of (PVA-BaTiO₃-TiO₂) nanocomposite.

4.4.3 The A.C Electrical Conductivity of (PVA-BaTiO₃-TiO₂) nanocomposites.

Figure (4.18) show the relationship between A.C electrical conductivity and concentration of (BaTiO₃-TiO₂) nanoparticles, with barium titanate and titanium dioxide concentration at 100Hz. The conductivity is increasing with the increase of barium titanate and titanium dioxide nanoparticles concentration. This increase is due to the effect of the space charge and the formation of a continuous network from barium titanate and titanium dioxide nanoparticles inside the nanocomposites [112].

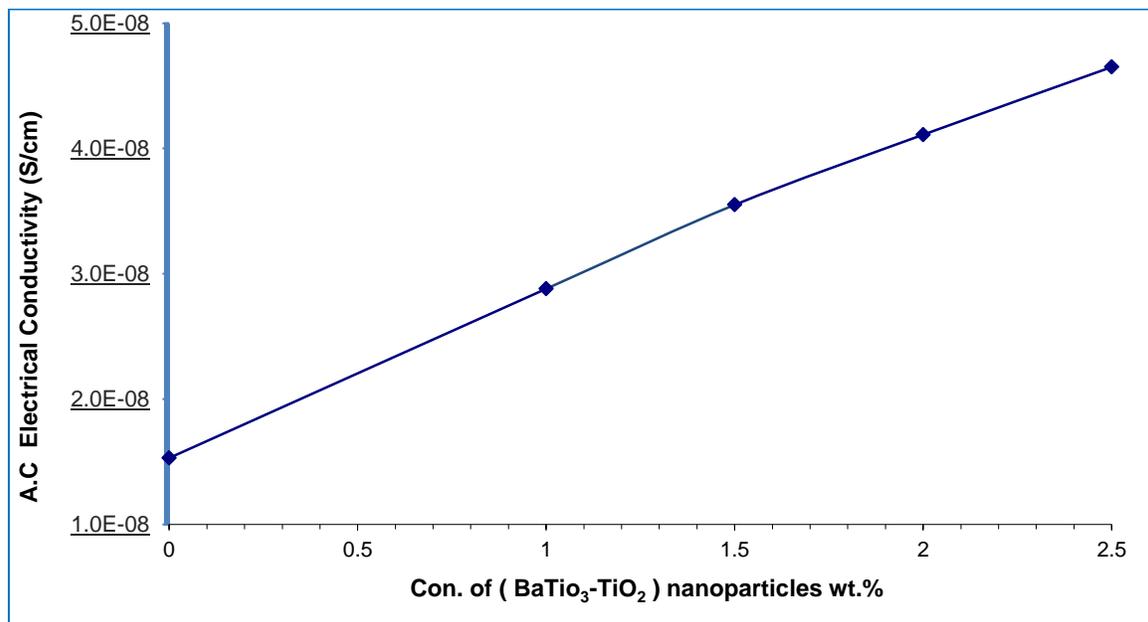


Figure (4.18) Relationship between A.C electrical conductivity and concentration of (PVA-BaTiO₃-TiO₂) nanocomposites.

Figure (4.19) shows relationship between A.C electrical conductivity and frequency of (PVA-BaTiO₃-TiO₂) nanocomposites. The figure shows that A.C conductivity increases considerably with the increase of frequency, this is attributed to the space charge polarization that occurs at low frequencies, and to the motion of charge carriers by the hopping process. The increase of the

conductivity is small at high frequencies because of the electronic polarization and the charge carriers that travel by the hopping process [112]. Consequently, the conductivity is increasing when increasing the frequency for all different ratio of barium titanate and titanium dioxide nanoparticles for (PVA-BaTiO₃-TiO₂) nanocomposites.

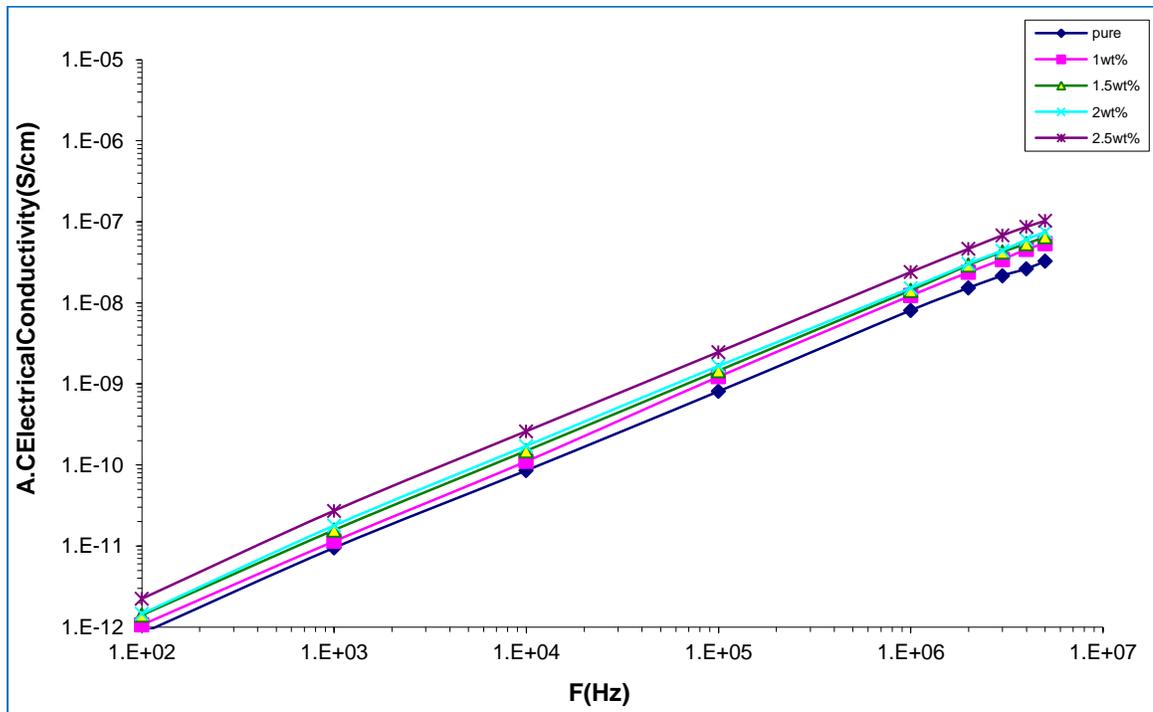


Figure (4.19) Relationship between A.C electrical conductivity and frequency of (PVA-BaTiO₃-TiO₂) nanocomposites.

4.5-Applications of (PVA-BaTiO₃-TiO₂) Nanocomposites for Antibacterial Activity

Figure (4.21) the inhibition zone for nanocomposites films was greater in Gram-negative (*Escherichia coli*) compounds than in Gram-positive bacteria. The width of the inhibition zone rises with increasing BaTiO₃ and TiO₂ concentration and reaches its maximum value (25mm) for Gram-negative (*Escherichia coli*) compounds with the greatest BaTiO₃ and TiO₂ content (2.5 wt.%). This result

suggests that nanocomposite films suppress the development of *Escherichia coli* and *Staphylococcus aureus*. Oxidative stress caused by reactive oxygen species (ROS) may be the primary mechanism behind the antibacterial activity of nanoparticle-based nanocomposites films. ROS contains radicals such as superoxide radicals (O_2^-), hydroxyl radicals ($-OH$), and hydrogen peroxide (H_2O_2); and singlet oxygen may be responsible for causing damage to the bacteria's proteins and DNA ($1O^2$). The current (PVA-BaTiO₃-TiO₂) nanocomposites exhibit the greatest antibacterial action against *Staphylococcus aureus* and *Escherichia coli*, are shown in figure (4.20) which is attributed to the high antibacterial activity of BaTiO₃ and TiO₂ nanoparticles [113,114,115].



(E. coli)



(Staph)

Figure (4.20) Image for inhibition zones of (PVA-BaTiO₃-TiO₂) nanocomposite films on *S. aureus* and *E. coli*.

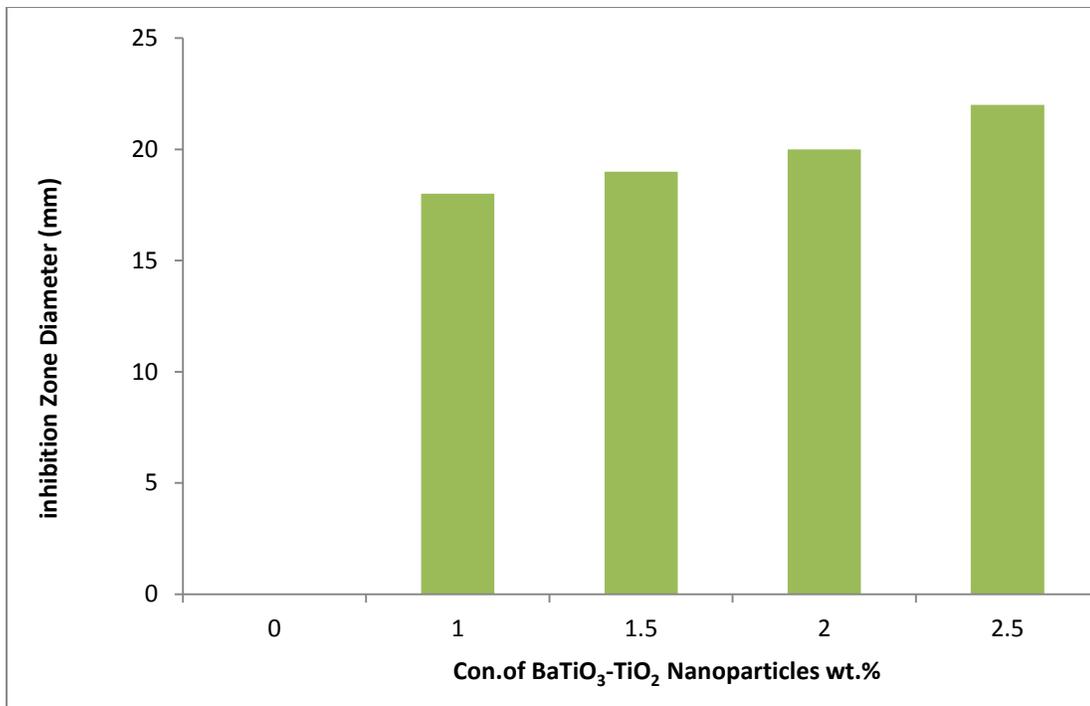


Figure (4.21) Variation inhibition zone diameter of (PVA- BaTiO₃-TiO₂) nanocomposite films for *E. coli* with concentration of (BaTiO₃-TiO₂) nanoparticles.

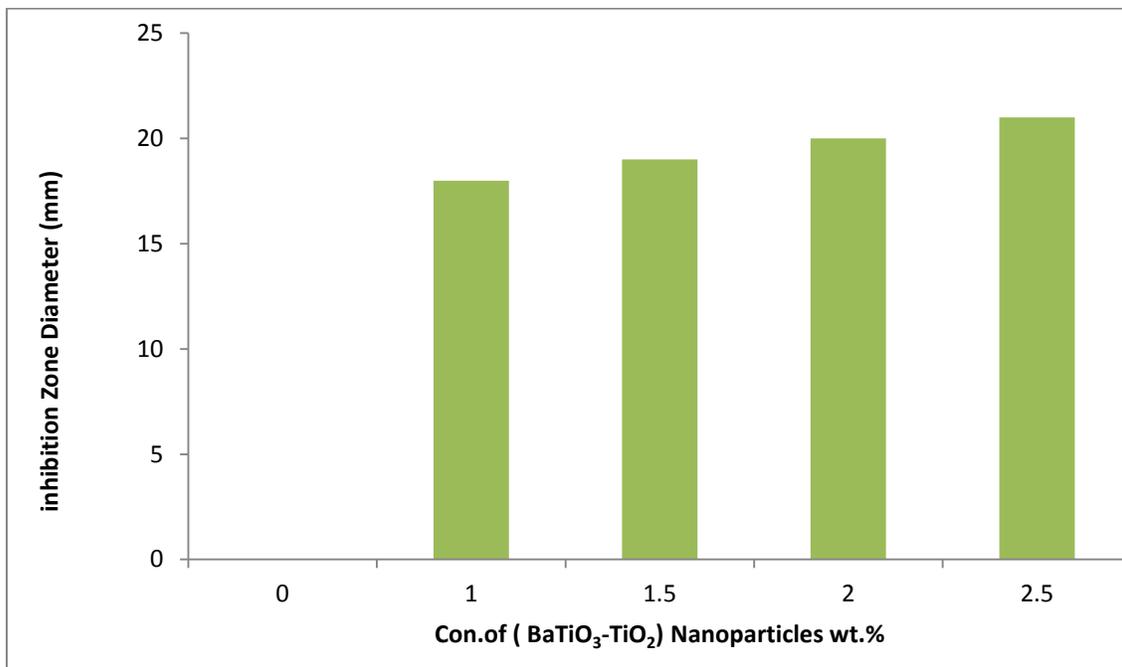


Figure (4.22) Variation inhibition zone diameter of (PVA- BaTiO₃-TiO₂) nanocomposite films for *S. aureus* with concentration of (BaTiO₃-TiO₂) nanoparticles.

4.6 Conclusions

From the obtained results and discussions, the following points are concluded:

- 1- The barium titanate and titanium dioxide nanoparticles from a continuous network within the nanocomposites were visible using an optical microscope at a concentration of (2.5wt.%). The FTIR spectra reveals variations in certain bands and improvements in the intensities of others as compared to pure (PVA) films. This indicates the considerable not the interaction between the polymer and($\text{BaTiO}_3\text{-TiO}_2$) nanoparticles.
- 2- SEM measurements reveal the surface morphology of the (PVA- $\text{BaTiO}_3\text{-TiO}_2$) nanocomposites films, which are homogeneous and coherent with aggregates or chunks scattered at random on the top surface.
- 3- The absorbance of (PVA- $\text{BaTiO}_3\text{-TiO}_2$) nanocomposite increases as the concentrations of($\text{BaTiO}_3\text{-TiO}_2$) nanoparticles increase, while the transmittance and energy gap of (PVA- $\text{BaTiO}_3\text{-TiO}_2$) nanocomposite decrease with increase concentrations of ($\text{BaTiO}_3\text{-TiO}_2$) nanoparticles.
- 4- The absorption coefficient, extinction coefficient, refractive index, real and imaginary parts of dielectric constants and optical conductivity are increasing with the increase of the weight percentages of barium titanate and titanium dioxide nanoparticles.
- 5- The dielectric constant, dielectric loss, and A.C electrical conductivity of (PVA- $\text{BaTiO}_3\text{-TiO}_2$) nanocomposites an increases with increase in the concentrations of($\text{BaTiO}_3\text{-TiO}_2$) nanoparticles, while dielectric constant and dielectric loss are decreasing as frequency increases, also A.C electrical conductivity increases with an increase in the frequency.

6-The inhibition zone for gram-positive and gram-negative was increased with increase the concentrations of BaTiO₃ and TiO₂ nanoparticles.

4.7 Future Works

1- Studying the effect of radiation on some physical properties of (PVA- BaTiO₃- TiO₂) nanocomposites.

2-Studying the thermal and mechanical properties of (PVA-BaTiO₃) nanocomposites, and Studying the rheological properties of (PVA -TiO₂) nanocomposites

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الخلاصة

تم تحضير المتراكبات النانوية (PVA-BaTiO₃-TiO₂) بطريقة صب المحلول بتراكيز (0,1,1.5,2 and 2.5) wt.%. تم دراسة الخصائص التركيبية والبصرية والكهربائية للمتراكبات النانوية. وتتضمن الخصائص التركيبية الأشعة تحت الحمراء لتحويل فوريير (FTIR) ، والمجهر الإلكتروني الماسح (SEM) والمجهر الضوئي (OM). أظهرت نتائج صور المجهر الضوئي و SEM توزيع جسيمات تيتانات الباريوم و ثاني أكسيد التيتانيوم النانوية داخل البوليمر. ويكشف المجهر البصري أيضًا أن الجسيمات النانوية داخل البوليمرات تكون شبكة مستمرة متصلة عند التراكيز العالية. أظهرت نتائج (FTIR) أن جميع قمم معظم الروابط تبقى في نفس موقع الاعداد الموجية. أظهرت نتائج الخواص البصرية للمتراكبات النانوية (PVA-BaTiO₃-TiO₂) أن الامتصاصية ومعامل الامتصاص ومعامل الخمود ومعامل الانكسار وثابت العزل الحقيقي والخيالي والتوصيلية البصرية تزداد بزيادة تراكيز الجسيمات النانوية BaTiO₃ و TiO₂ بينما النفاذية و فجوة الطاقة تقل مع زيادة تراكيز الجسيمات النانوية BaTiO₃ و TiO₂. وتحتوي المتراكبات النانوية على مستوى عال من امتصاص لأشعة فوق البنفسجية. أظهرت نتائج الخواص الكهربائية المتناوبة للمتراكبات النانوية أن ثابت العزل وفقدان العزل الكهربائي لهذه المتراكبات النانوية تنخفض مع زيادة تردد المجال الكهربائي المسلط ، وتزداد مع زيادة تراكيز جسيمات BaTiO₃ و TiO₂ النانوية ، بينما تزداد التوصيلة الكهربائية مع زيادة تراكيز جسيمات BaTiO₃ و TiO₂ النانوية. أظهرت نتائج التطبيقات المضادة للبكتيريا للمتراكبات النانوية (PVA-BaTiO₃-TiO₂) زيادة منطقة التثبيط للمركبات النانوية الموجبة والسالبة للجرام مع زيادة تراكيز الجسيمات النانوية BaTiO₃ و TiO₂.



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