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Optical and Electrical characterization of Polystyrene doped with Iron Oxide Nanoparticle

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Abstract: *In this paper, simple and inexpensive method for preparation of different concentrations of polystyrene doped with iron by sol-gel method.* Fe_2O_3*/PS nanoparticles with different concentration (0.5%,1% and2%) were characterized by using X-ray Diffraction (XRD), Ultraviolet and Visible regions (UV-Vis) are studied in ranged (200-800)nm and Electrical properties at temperature range from (303-403)K.*

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I. Introduction:

A polymer(1,2) is large molecule composed of many repeated subunits, known as monomers because of their broad range of properties(3), both synthetic and natural polymers play an essential and ubiquitous role in everyday life(4). Polymers range from familiar synthetic plastic such as polystyrene (or Styrofoam) to natural bio-polymers such as DNA and proteins that are fundamental to biological structure and function. Polymers, both natural and synthetic, are created via of polymerization many monomers. Their consequently large mass relative to small molecule compounds produces unique physical properties, including toughness, viscoelasticity, and a tendency to form glasses and semi crystalline structures rather than crystals.

Polystyrene is a synthetic aromatic polymer made from the monomer styrene, a liquid petrochemical. Polystyrene can be rigid or foamed. General purpose polystyrene is clear, hard and brittle. It is a very inexpensive resin per unit weight. It is a rather poor barrier to oxygen and water vapor and has a relatively low melting point (4) Polystyrene is one of the most widely used plastics, the scale of its production being several billion kilograms per year.(5) Polystyrene can be naturally transparent, but can be colored with colorants. As a thermoplastic polymer, polystyrene is in a solid (glassy) state at room temperature but flows if heated above about 100 °C, its glass transition temperature. It becomes rigid again when cooled. This temperature behavior is exploited for extrusion, and also for molding and vacuum forming, since it can be cast into molds with fine detail. Polystyrene (PS) is used for producing disposable plastic cutlery and dinnerware, CD “jewel” cases, smoke detector housings, license plate frames, plastic assembly kits, and many other objects where a rigid, economical plastic is desired. Polystyrene Petridishes and other laboratory containers such as tube sand micro plates play an important role in biomedical research and science.

Iron oxides are one of the most important transition metal oxides of technological importance, it exist in nature in many forms in which magnetite (Fe_3O_4), maghemite (γ-Fe_2O_3) and hematite (α-Fe_2O_3) are probably the most common(6). Hematite (α-Fe_2O_3) is the oldest oxide and is widespread in rocks and soils. It is the most stable iron oxide under ambient condition and has significant scientific and technological importance(7). The stability and semiconductor (n-type) properties of α-Fe_2O_3 allow it to be used as a photocatalyst. Currently the α-Fe_2O_3 photo electrode has received considerable attention as a solar energy conversion material due to its excellent properties, such as a small band gab (2.1 eV), high resistivity to corrosion and low cost(8). Also magnetic nanoparticles have shown great potential application in cancer cell killing (9). Magnetite and maghemite have attraced attention in biomedical applications because of their biocompatibility water soluble and low toxicity in the human body(10-13).

II. Experimental:

2.1 Materials

Polystyrene Chemical pure, $(C_8H_8)_n$ M_{wt} = 280, Ferric chloride hexahydrate $FeCl_3.6H_2O$, M_{wt} = 270.30 g mol^{-1} and Methanol CH_3OH, M_{wt} = 30.04 g mol^{-1}, Sodium hydroxide NaOH, M_{wt} = 39.997 g mol^{-1}, Ferrous chloride hexahydrate $FeCl_2.6H_2O$, M_{wt}= 126.751 g mol^{-1}.

2.2 Synthesis of PS:

1 gm of Polystyrene was dissolved in 10 ml of toluene using hot plate magnetic stirrer at 50° C for 1 hr to obtain homogeneous solution.(14)

2.3 Synthesis of Fe_2O_3 Nanoparticles:

In the present work, Iron oxide nanoparticles were synthesis by sol-gel process with iron chloride hexahydrate ($FeC1_3.6H_2O$) as the Fe source. In typical experiments, 1.693 g of $FeCl_3.6H_2O$ was added to 50 ml of methanol and stirred at 60°C for 1 h to form a gel. The heating was stopped and the solution was stirred continuously until a brownish colored powder formed. The powder was filtered and washed repeatedly with methanol and dried. The dried powder was sintered in a furnace at 700^o C for 1 h to obtain a nanocrystalline Fe_2O_3 powder [(15)].

2.4 Synthesis of Fe_2O_3/Ps Nanoparticle Films:

Fe_2O_3/PS nanoparticles were prepared by adding nano.Fe_2O_3 in different weight (0.5%, 1% and 2%) to polystyrene solution and the mixture was stirrer for 2hr while keeping to the temperature constant at 50°C.

III. Methods:

The prepared samples were identified by means of X-ray diffraction (XRD) using Copper target with Nickel filter. The samples were subjected to X- ray analysis under working conditions of 40 kV and 20 mA. The measurement of the UV- Visible spectra were carried out on UV1600/1800 series spectrophotometer with spectra range (200-800) nm. The Ac electrical conductivity of the prepared samples had been measured over the temperature range from (303-403)K and frequency range (100 -1200)KHz using LCR Bridge Hioki 3531 Z Hitester "Japan".

IV. Results and Discussion:

4.1. (XRD) measurements:

The XRD pattern of nano. Fe_2O_3 is shown in figure (1). Eleven peaks observed in the XRD pattern of nano. Fe_2O_3 at 2θ = 24.16°, 33.11°, 35.62°, 40.86°, 49.46°, 54.11°, 57.60° ,62.34°, 64.02°, 71.89° and 75.34° respectively. These peaks were corresponding to (012), (104), (110), (113), (024), (116), (018), (214), (330), (101), and (220) plans of hexagonal structure Fe_2O_3 respectively. The calculated particle size from the average of the prepared Fe_2O_3 is 16.7nm.

XRD pattern of pure polystyrene (PS) is shown in figure (2). The pattern show a broad peak of PS at 2θ = 19.65°, confirming the amorphous nature of polymer.

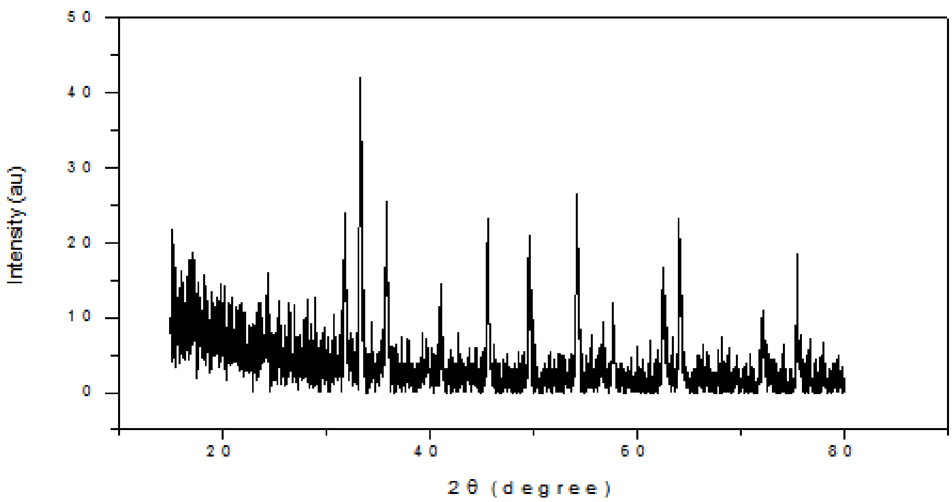

Figure (1): XRD pattern of Fe2O3 Nanoparticle.

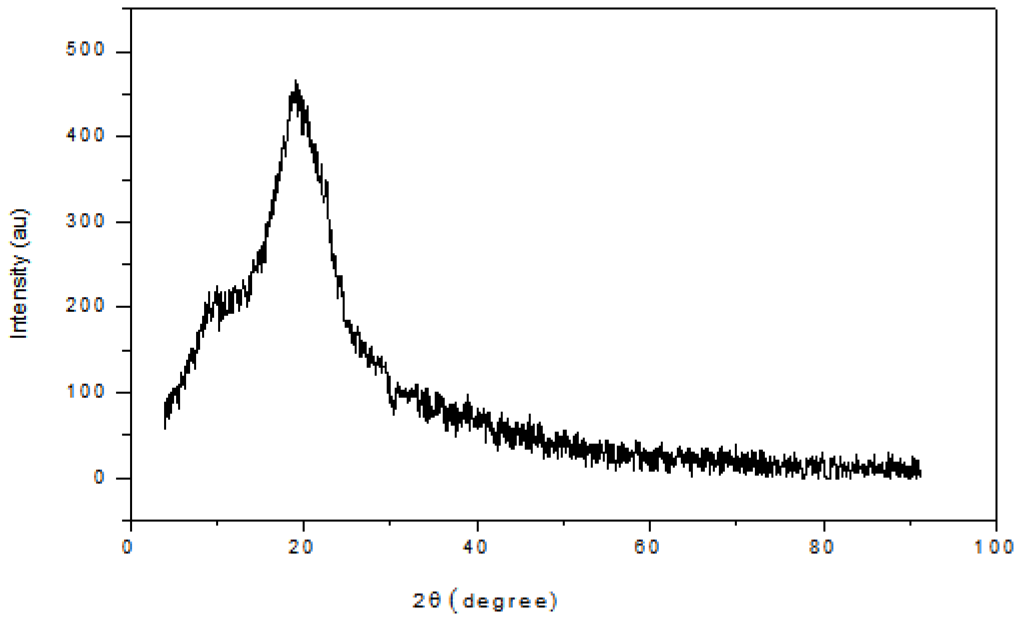

Figure (2): XRD pattern of pure polystyrene

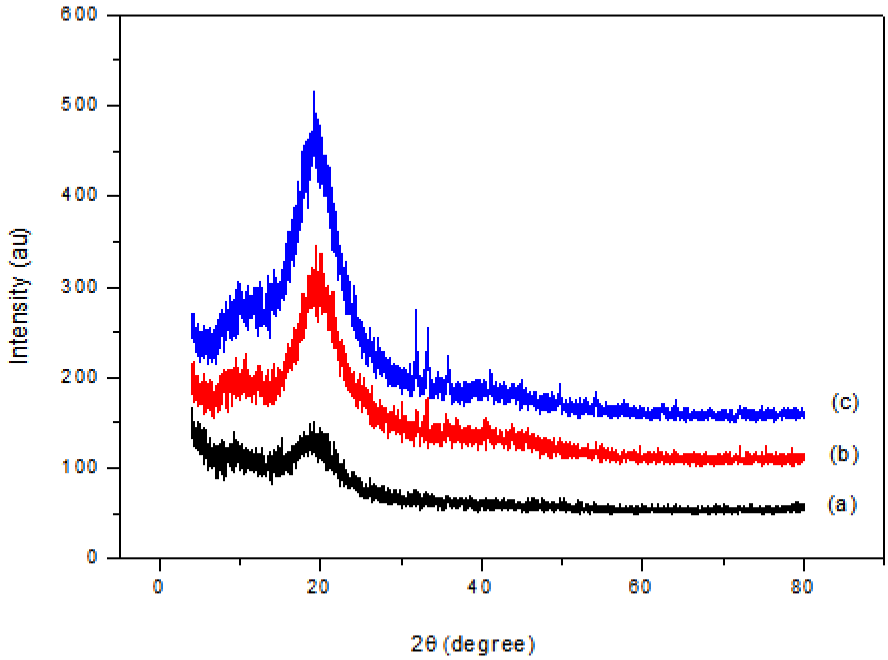

Figure (3): XRD patterns of nano. Fe_2O_3 /PS with different Concentration, (a) 0.5% Fe_2O_3/PS, (b) 1% Fe_2O_3/PS and (c) 2% Fe_2O_3.

The XRD pattern of nano.Fe_2O_3/PS film with different concentration (0.5%,1% and 2%) are shown in figure (3). The pattern showed more intense and crystalline diffraction peaks of Fe_2O_3/PS appeared at $2\theta = 33.11°$. The diffraction peak for Fe_2O_3/PS become sharper and more intense by increase the concentration of nano. Fe_2O_3, this result indicated that PS has influence on crystalline of nano.Fe_2O_3 [16].The particle size for nano. Fe_2O_3/PS with different concentration (0.5%, 1% and 2%) are (17.83, 18.94 and 21.25)nm respectively.

4.2: UV- Visible Spesctroscopy:

UV-Vis absorption spectra of pure polystyrene and polystyrene doped with nano. Fe_2O_3 at different concentrations (0.5%,1%,2%) are shown in figure (4:a,b,c,d). By comparing the electronic spectrum of pure polystyrene with electronic spectrum of doped with nano. Fe_2O_3,it was observed that the peak at 246nm for pure

Ps which assigned to π-π^* transition is shifted to higher wavelength (265,267and269)nm by increasing concentrations of nano.Fe_2O_3 (0.5%,1%,2%) respectively. This may be attributed to the conjugation in the structure. Also it can be noticed that the absorbance increase with increasing the concentration of nano. Fe_2O_3 in the samples.

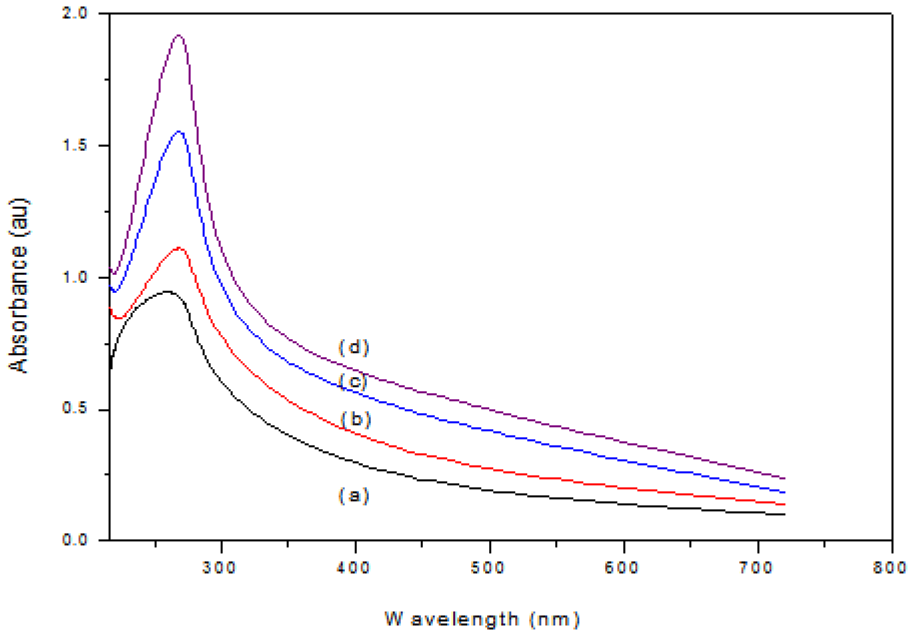

Figure (4:a,b,c,d)): UV-Visible spectra of pure polystyrene and Nano.Fe_2O_3/ PS at concentration (0.5%,1%,2%) respectively

4.3. The Optical Parameters:

The optical absorbance spectra (A), the absorbance coefficient and refractive index of nano. Fe_2O_3/PS films were studied at differernt concentration (0.5%.1% and 2%).The obtained spectra were recorded in wavelength range (190-2500) nm are shown in figures(5-8).

Fig (5) shows the absorption spectra of the prepared samples. It can be seen that the absorbance increases as the percentage of nano. Fe_2O_3 increases. Adding different concentration of filler material to the polymer do not change the chemical structure of the polymer but new physical properties to the mixture will formed. This result agree with previous studies[17].

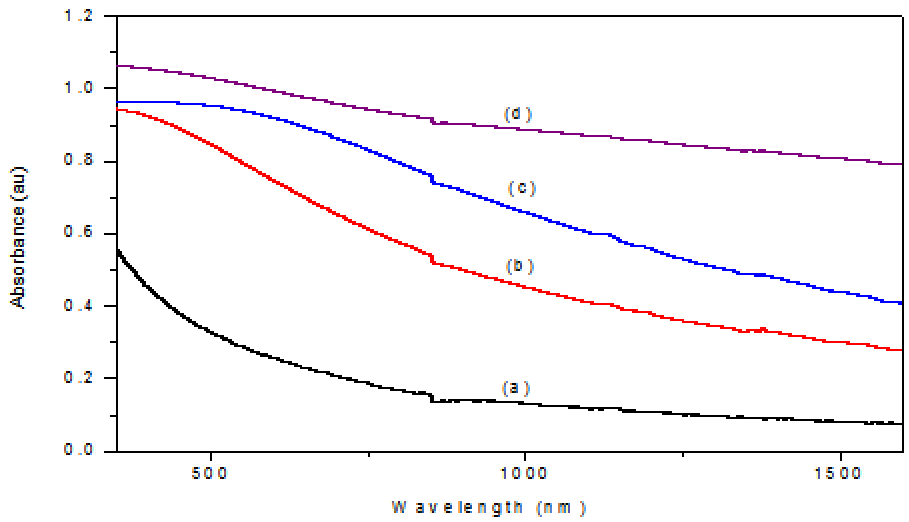

Figure (5): Variation of the absorbance against wavelength (a) Pure PS, (b) 0.5% Fe_2O_3/PS,1% % Fe_2O_3/PS and (d) 2% % Fe_2O_3/PS

Figure (6) show the relationship between the absorption coefficient and photon energy of nano. Fe_2O_3/PS It was observed that at high energy, absorption is great and the forbidden energy gap is less which indicates that the large probability of electronic transitions.

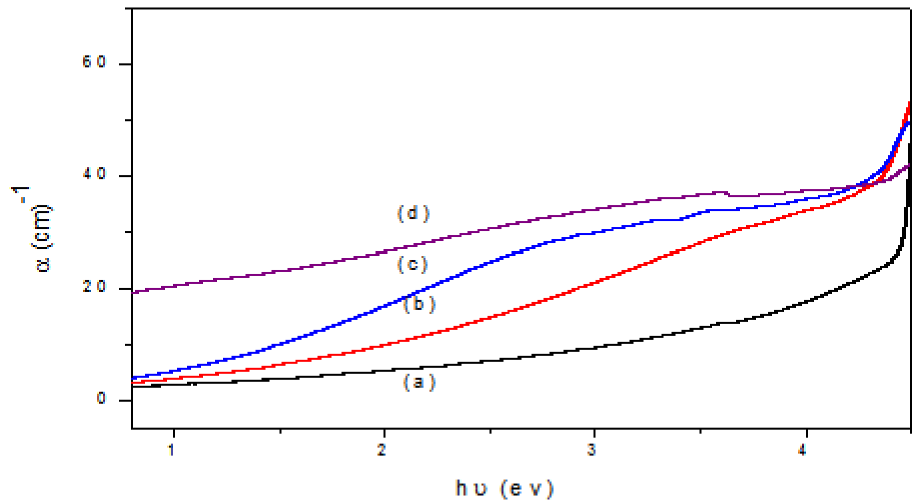

Figure (6): Variation of the absorbance coefficient against hυ (a) Pure PS, (b) 0.5% Fe_2O_3/PS, (c) 1% Fe_2O_3 /PS and (d) 2% Fe_2O_3/PS.

The variation of refractive index with respect to wavelength of nano Fe_2O_3 /PS have been shown in figure (7) it have been observed that refractive index of polystyrene increases with increasing nanoparticles wt%. So this type of the doping polymer can be used in wave guide technology (e.g. planar waveguide and optical fiber), anti refractive coating, photonic devices, solar cells and image sensor [18,19].

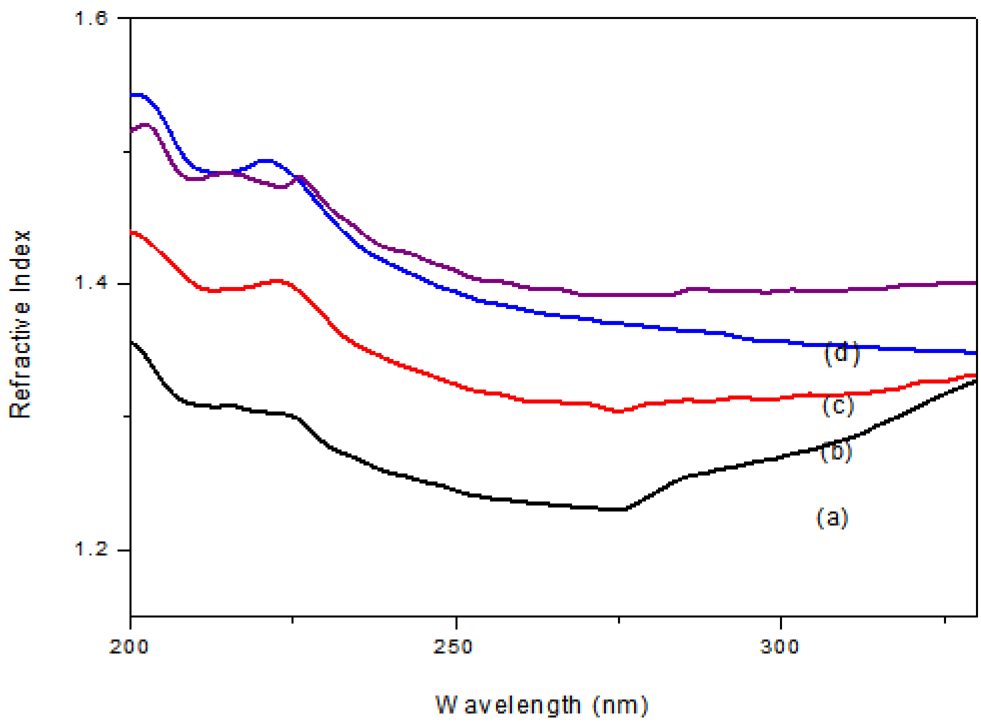

Figure (7): Variation of the refractive index against wavelength (a) Pure PS, (b) 0.5% Fe_2O_3/PS, (c) 1% Fe_2O_3/PS and (d) 2% Fe_2O_3/PS.

Figure (8) shows that, the variation of the optical energy gap for nano. Fe_2O_3/PS against the photon energy. It can be observed that curve is characterized by the presence of an exponentially decaying tail at low photon energy, thus the optical energy gap decreased with increasing dopant concentration.

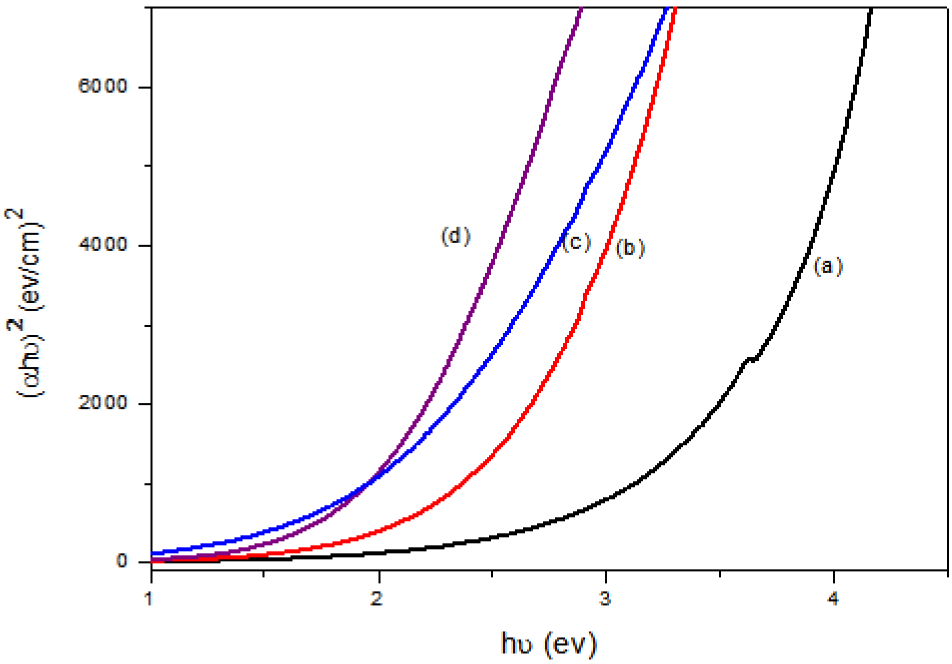

Figure (8): Vartion $(\alpha h\nu)^2$ of the against (hν)(a) Pure PS, (b) 0.5% Fe_2O_3/P (c) 1% Fe_2O_3/PS and (d) 2% Fe_2O_3/PS.

4.4: Electrical Conductivity Studies:

The electrical conductivity of polystyrene and polystyrene doped with nano.Fe_2O_3 at different conc. (0.5%, 1% and 2%) were investigated over the temperature range from room temperature to about 403 K.

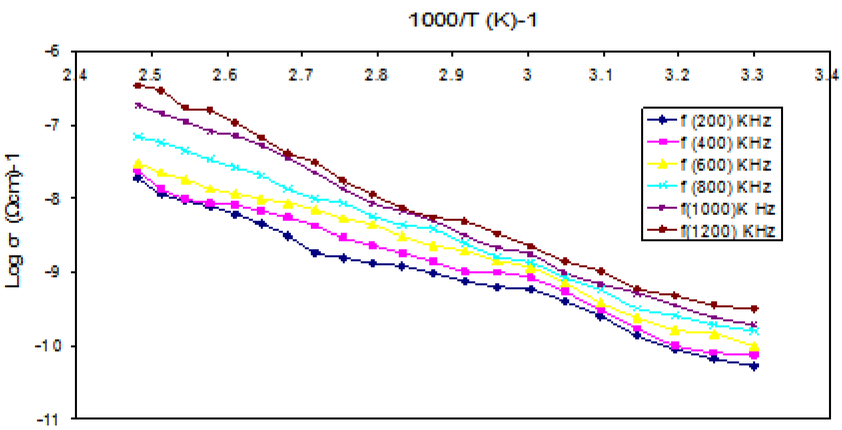

Figure (9): The variation of log σ (AC Conductivity) with 1000/T for polystyrene measured at different frequencies

The dependance of electrical conductivity on the recipocal of absolute temperature at different frequencies ranging from (100-1200) KHz for the pure and doped polystyrene with Fe_2O_3 at different concentration are shown in figures from (9-12). From this figures it can be noticed that ,the electrical conductivity increases with increasing temperature.This increase can be assigned to two factors [20], the increase in the mobility of charge carriers and the increase in the rate of charge carrier's generation.

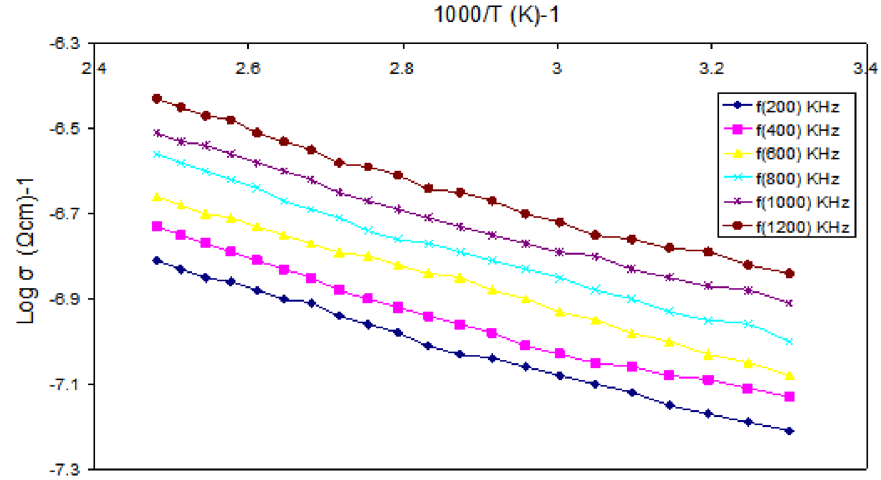

Figure (10): Variation of log σ (AC Conductivity) with 1000/T for 0.5%Fe_2O_3/PS measured at different frequencies

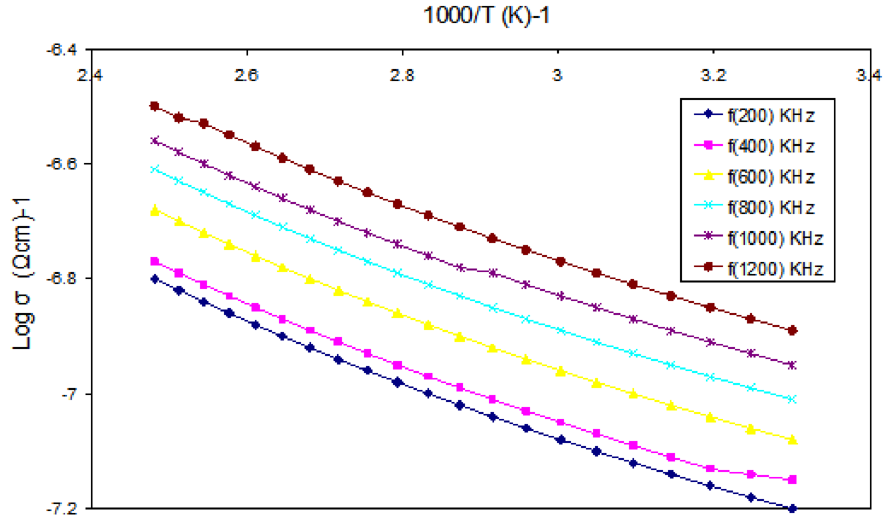

Figure (11): Variation of log σ (AC Conductivity) with 1000/T for 1% Fe_2O_3/PS measured at different frequencies

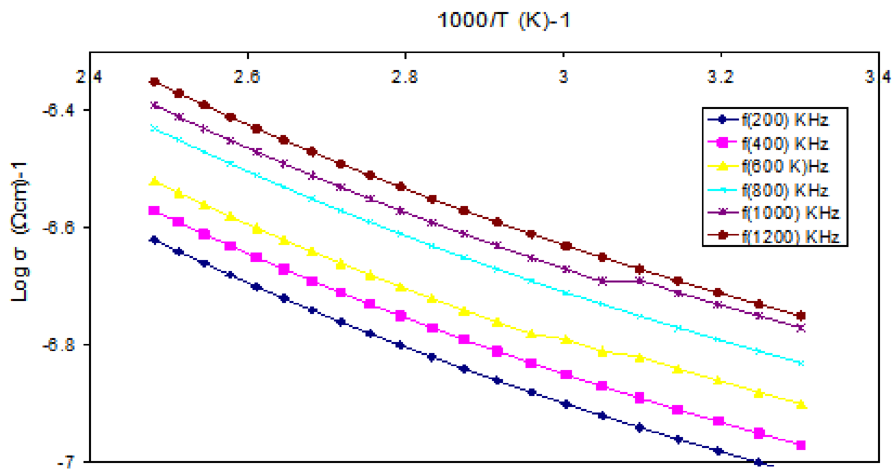

Figure (12): Variation of log σ (AC Conductivity) with 1000/T for 2% Fe_2O_3/PS at different frequencies

The variation of dielectric constant of pure polystyrene and polystyrene doped with Fe_2O_3 nanoparticles at different concentrations (0.5% ,1% and 2%) as a function of frequency range from (200 to 1200) KHz and measured at different temperatures (303-403)K are shows in figures (13-16).

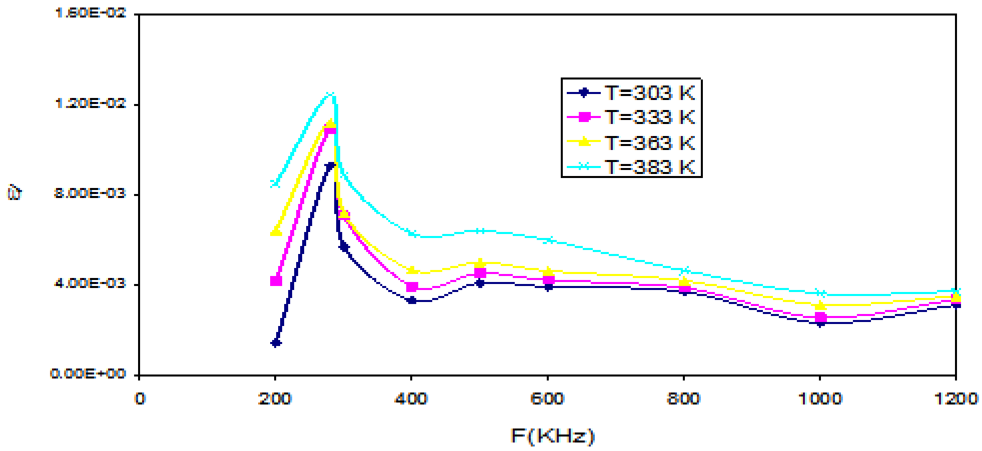

Figure (13): Variation of dielectric constant of polystyrene as function of frequency at different temperature.

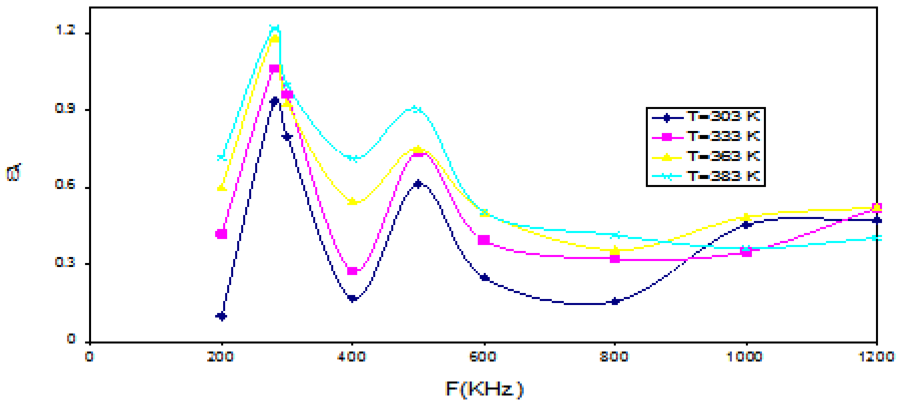

Figure (14): Variation of dielectric constant of 0.5% Fe_2O_3/PS as function of frequency at different temperature

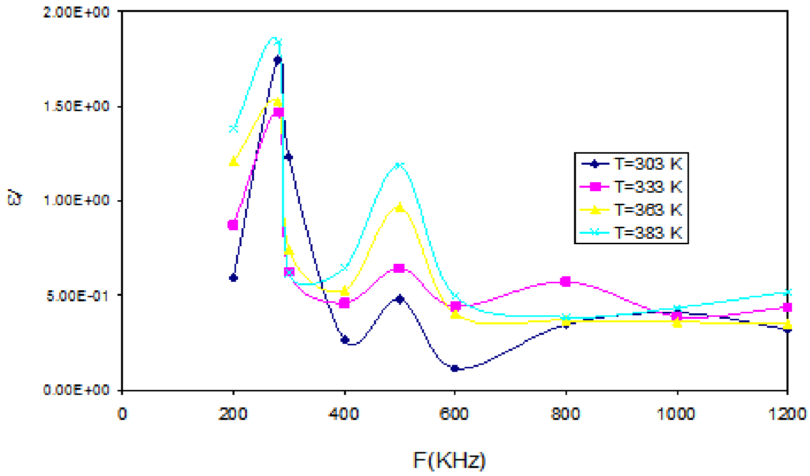

Figure (15): Variation of dielectric constant of 1% Fe_2O_3/PS as function of frequency at different temperature.

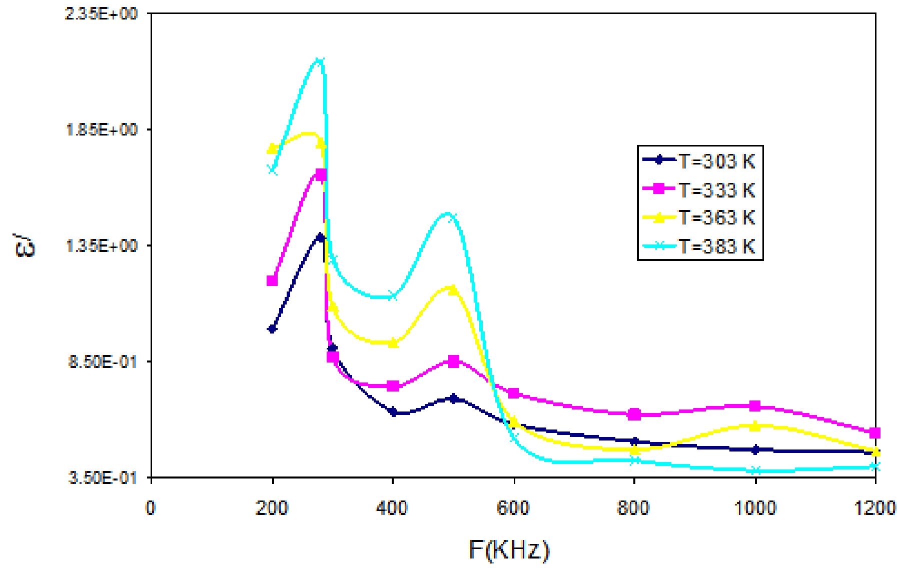

Figure (16): Variation of dielectric constant of 2% Fe_2O_3/PS as function of frequency at different temperature.

From this figures it can be seen that each ε′ curve contains two maximum peaks; one around lower frequency at 280 KHz and the other higher frequency at 500 KHz. The permittivity of polystyrene increases, with increasing temperature,this attributed to the orientation of dipoles which formed from the charge carriers.On the other hand the decrease in dielectric constant with frequency for investigated samples at given temperature may be attributed mainly to the decreasing number of dipoles which contribute to polarization.

Figures (17 -20) represent the change of imaginary part of dielectric constant (ε") for pure polystyrene and polystyrene doped with different concentration of Fe_2O_3 nanoparticles with frequency range (200-1200) KHz, at different temperature range (303-403) K.

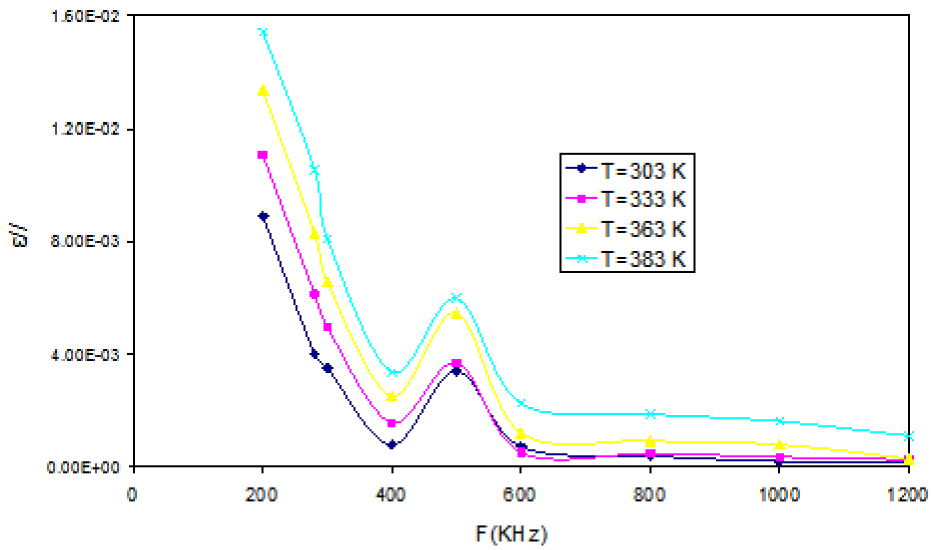

Figure (17): Variation of dielectric loss of Polystyrene
as function of frequency at different temperature.

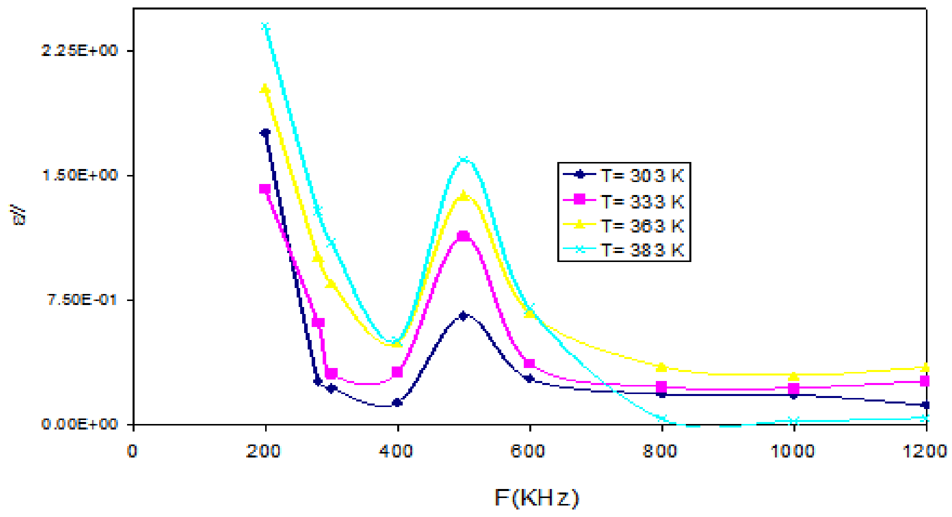

Figure (18): Variation of dielectric loss of 0.5%Fe_2O_3/PS as function of frequency at different temperature

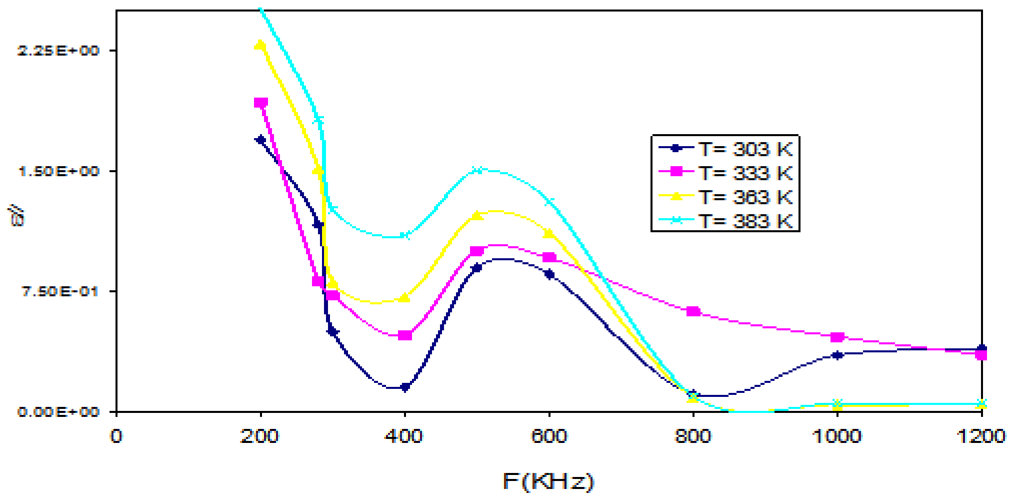

Figure (19): Variation of dielectric loss of 1%Fe_2O_3/PS as function of frequency at different temperature

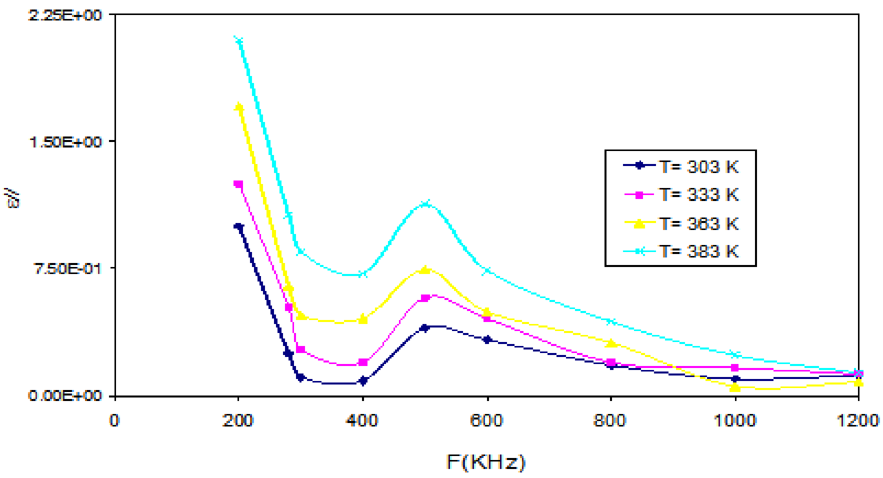

Figure (20): Variation of dielectric loss of 2%Fe_2O_3/PS as function of frequency at different temperature.

From the figures, it can be seen that ε" was decrease with increasing frequency until reached at maximum peak of frequency (500)KHz for all samples. This may be attributed to the increased of mobility of polar groups and increase in the number of mobile dipoles at this frequency[21], then ε" decrease again with increasing frequency ubtill (1200) KHz. It can be observed that a shift of maximum dielectric loss ε" toward higher frequencies as the temperature increases. This related to the increase of the mobility of polar groups and increase the number of mobile dipoles.

V. Conclusion:

In this work Iron Oxide nanoparticles was prepared by sol gel method then doped with polystyreen at different concentrations(0.5,1, and 2%). In this thesis XRD, UV,Optical properties and Electrical properties were studied.From XRD pattern of polystyreen doped with different concentration of Fe_2O_3 nanoparticles shows that the particle size of Fe_2O_3/PS are (17.8,18.9,21.2 nm)for (0.5,1,2%)of Fe_2O_3 respectively.The UV-Visible spectra shows that the band shifted to higher wavelenght in doped polystyreen due to the extent of conjugation of the work structure. The electrical conductivity of pure polystyreen and doped polystyrene were measured at different temperatures, from results it can be found the conductivity increse with increasing temperature which indicate the materials are semiconductor in nature. **"Data Availability"**

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