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Comparison Between Electronic and Optical Band Gap Polyindole/Poly(Vinyl Acetate) Composite

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Abstract

In present research work, comparison between electronic and optical band gap of polyindole/poly(vinyl acetate) (PIN/PVAc) composite are reported. The synthesized composite was analyzed via DC conductivity measurement and UV–Visible spectroscopy. The value of DC conductivity primarily increases and reaches to 1.89×10^{-6} S/cm at 383 K. The value of electronic and optical band gap of composite is established as 2.831 eV and 3.81 eV respectively. The semiconducting nature of PIN/PVAc composite reflects from electronic and optical band gap and Arrhenius behaviour of DC plot.

Keywords: Polyindole/poly(vinyl acetate); composite; electronic; optical; band gap.

Introduction

Conducting polymer composites develop into the novel and attractive group of materials due to their superior properties. They have fascinated a lot concern due to its unique optical and electrical properties in addition to its superior thermal stability. Polyindole has received excellent research interest because of its close structural similarities with both polyaniline and polypyrrole. Also, due to its extraordinary conduction mechanism and environment stability as compared to other conducting polymers [1-7]. Some researchers were given so much attention for synthesizing the polyindole composite materials due to its amazing properties. Researchers such as Koyuncu et al. studied the opportunity of preparing a colloidal steady poly(vinyl chloride)/polyindole ER active composite system [8]. Sari et al. presented preparation, characterization, ER and creep–recovery properties of polyindole/polyethylene composites [9].

This research paper gives the information about the comparison between electronic and optical band gap of polyindole/poly(vinyl acetate) (PIN/PVAc) composite which is chemically prepared using ferric chloride as a oxidant. As–synthesized composite was characterized through DC conductivity measurement technique and ultraviolet–visible (UV–Vis) spectroscopy.

Experimental

All chemicals used in this research were of AR grade and procured from SD Fine Chemicals, India, like as monomer indole, oxidant ferric chloride ($FeCl_3$), organic media methanol. Polyvinyl acetate (PVAc) (Himedia Chemicals, India) used as counter polymer.
The polyindole/poly(vinyl acetate) (PIN/PVAc) composite was synthesized through chemical polymerization route using oxidant $FeCl_3$. Poly(vinyl acetate) (1 g) was dissolved in methanol (9 ml) and stirred 2 h then kept solution for 24 h to get homogenous solution. The monomer indole (0.5 g) was added in PVAc solution and stirred for 2 h. The indole was chemically polymerized using oxidizing agent $FeCl_3$ (0.1097 g) and stirred it for 2 hr to complete polymerization process. Then reaction mixture was kept for 60 min to settle down. Then composite solution was poured

on dry and cleaned glass plate. To dry the film by an isothermal evaporation of organic media, complete assembly was placed for 24 h in dust free chamber kept at constant temperature. After that film was washed with double distilled water and takes out from glass plate then dried out for 6 h at room temperature. In that way, PIN/PVAc composite was synthesized chemically.

As–synthesized composite was characterized through UV–VIS spectroscopy (Agilent Technologies, Cary 60 UV–VIS). The DC conductivity measurement was done through two probe technique.

Results and discussions

Dc Conductivity Results

The sample dimensions method is used to determined the DC conductivity. The temperature dependence of the DC conductivity for PIN/ PVAc composite in the temperature range 308–383 K shown in Fig. 1. The semiconducting nature of the synthesized composite is seen from Arrhenius behavior of plot in the figure and given by the relation [10].

$$\sigma_{DC} = \sigma_0 \exp(-E_{DC}/k_B T) \quad (1)$$

Where, σ_{DC} is DC conductivity, σ_0 is pre–exponential factor, E_{DC} is activation energy, T is absolute temperature and k_B Boltzmann's constant.

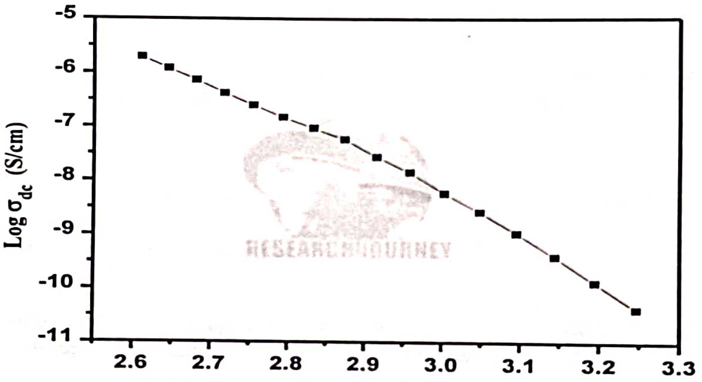

Fig 1. Temperature dependence DC conductivity.

The DC conductivity value of PIN/ PVAc composite is determined as 1.89×10^{-6} S/cm. The DC conductivity of composite is increase with increase in temperature, demonstrating negative temperature coefficient (NTC) of resistance. It shows that decrease in bulk resistance of sample. This typical improvement in conductivity owes to activate conduction mechanism. It seen that conductivity increase with increase in temperature, this can be because of the performance of PIN which triggered thermally. The conjugation length and chain alignment of conducting polymers demonstrates essential function of motion of charge carriers which affects DC conductivity. The activation energy decreases with raise in temperature and electric field outcome with charge carrier transportation. The diffusion of ions made effortless in space charge polarization by increasing temperature. To conquer activation barrier, thermal energy possibly support in direction of field to orientation of polar molecules [10-14].

Electronic and Optical Band Gap Determination

The electronic band gap is chief physical property that features a semiconducting material. The electronic band gap of PIN/PVAc composite can be determined by given equation [15],

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$$E_g = -2.303 \times 2k_B \times (slope) \times 10^3 \qquad (2)$$

Where, E_g is the electronic band gap, k_B is the Boltzmann's constant. The electronic band gap PIN/PVAc of sample is determined as 2.831 eV. The semiconducting nature of PIN/ PVAc composite is observed from electronic band gap values.

The Fig. 2 represents the UV–Vis spectrum of PVAc/PIN composite. The % absorption spectrum is examined in ultraviolet and visible range (200–560 nm). It is noticed that lower wavelength side shows superior % absorption as compared to higher wavelength side. It is studied that strongest absorption peak shows at wavelength 225 nm due to optical transition to conduction band from valence band.

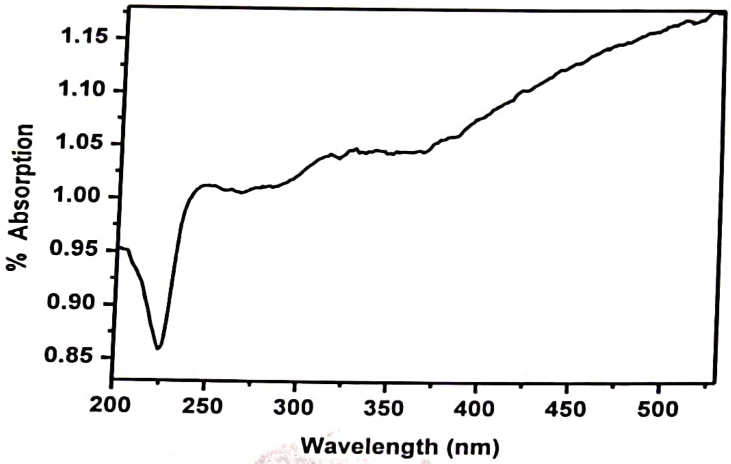

Fig. 2. UV–Vis spectrum.

The optical band gap value of PIN/PVAc composite is determined from plot of αhv versus photon energy (eV) as represent in the Fig. 2. The optical band gap value of composite could be determined from given expression [16].

$$\alpha = \frac{A(h\nu - Eg)^n}{h\nu} \qquad (4)$$

Where, hv is the incident photon energy, α is the absorption coefficient, A is the constant and Eg is the optical band gap of the material. The optical band gap of synthesized composite sample is determined as 3.81 eV. The optical band gap value of composite represents the application potential in optical devices and photo catalytic activities.

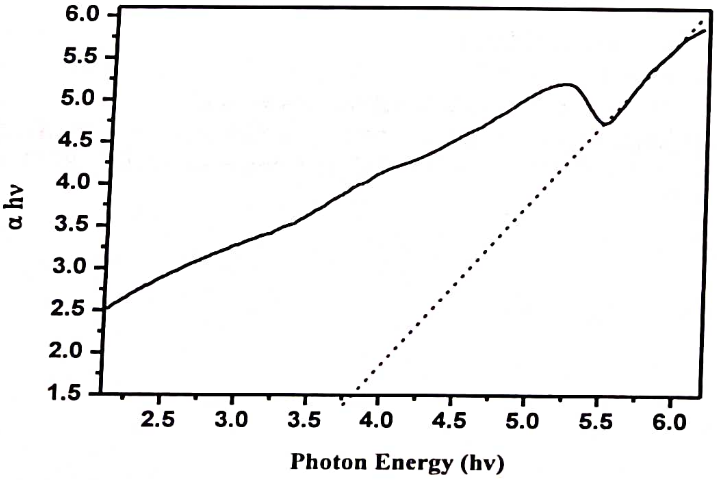

Fig. 3. Plot of photon energy versus αhv.

The comparison between the electronic and optical band gaps seen from their values which are calculated as 2.831 eV and 3.81 eV respectively. The electronic band gap is slightly less optical band gap observed from values. Also, the band gap values represent the semiconducting nature of PIN/PVAc composite material. The synthesized composite material has application potential in electronic as well as optical devices.

Conclusions

In summary, the electronic and optical band gap of composite is calculated as 2.831 eV and 3.81 eV respectively. The electronic band gap value reflects the composite have semiconducting properties. The value of optical band gap represents composite has potential application in optical devices.

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